From Relations to XML: Cleaning, Integrating and Securing Data

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Abstract

While relational databases are still the preferred approach for storing data, XML is emerging as the primary standard for representing and exchanging data. Consequently, it has been increasingly important to provide a uniform XML interface to various data sources — integration; and critical to protect sensitive and confidential information in XML data — access control. Moreover, it is preferable to first detect and repair the inconsistencies in the data to avoid the propagation of errors to other data processing steps. In response to these challenges, this thesis presents an integrated framework for cleaning, integrating and securing data.

The framework contains three parts. First, the data cleaning sub-framework makes use of a new class of constraints specially designed for improving data quality, referred to as *conditional functional dependencies* (CFDs), to detect and remove inconsistencies in relational data. Both batch and incremental techniques are developed for detecting CFD violations by SQL efficiently and repairing them based on a cost model. The cleaned relational data, together with other non-XML data, is then converted to XML format by using widely deployed XML publishing facilities. Second, the data integration sub-framework uses a novel formalism, XML *integration grammars (*XIG*s)*, to integrate multi-source XML data which is either native or published from traditional databases. XIGs automatically support conformance to a target DTD, and allow one to build a large, complex integration via composition of component XIGs. To efficiently materialize the integrated data, algorithms are developed for merging XML queries in XIGs and for scheduling them. Third, to protect sensitive information in the integrated XML data, the data security sub-framework allows users to access the data only through authorized views. User queries posed on these views need to be rewritten into equivalent queries on the underlying document to avoid the prohibitive cost of materializing and maintaining large number of views. Two algorithms are proposed to support virtual XML views: a rewriting algorithm that characterizes the rewritten queries as a new form of automata and an evaluation algorithm to execute the automata-represented queries. They allow the security sub-framework to answer queries on views in linear time.

Using both relational and XML technologies, this framework provides a uniform approach to clean, integrate and secure data. The algorithms and techniques in the framework have been implemented and the experimental study verifies their effectiveness and efficiency.

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Declaration

I declare that this thesis was composed by myself, that the work contained herein is my own except where explicitly stated otherwise in the text, and that this work has not been submitted for any other degree or professional qualification except as specified.

(*Xibei Jia*)

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Chapter 1

Introduction

Since the 1970s, relational databases have been widely used in managing large volumes of data. Whenever you call a friend, withdraw some money or book a flight, relational databases are working behind the scene. With the wide adoption of relational databases, more and more data has been accumulated and becomes one of the most valuable assets of an organization. The value of the data heavily relies on its *usability*. Unfortunately, the data in real-world organizations often has various problems which prevent it being used directly.

1.1 Real-world data is dirty, distributed and sensitive

Traditional database technologies are designed for the settings in which data is stored in well designed database management systems. However, in modern organizations, with the ubiquity of electronic information, the data is distributed in far more diverse information systems with various capabilities, including relational or object-oriented databases, XML repositories, content management systems, etc. The following example demonstrates the complexity of the data in a real world organization.

Example 1.1: Consider an automobile company which has accumulated a large volume of data in its operations. As illustrated in Figure 1.1, this data includes the information about its employees, customers, sales, products and services. Among them, the sales data is kept in a centrally managed database, which is evolved from the legacy systems running on the mainframe at the headquarter. The management of other data is far more complex.

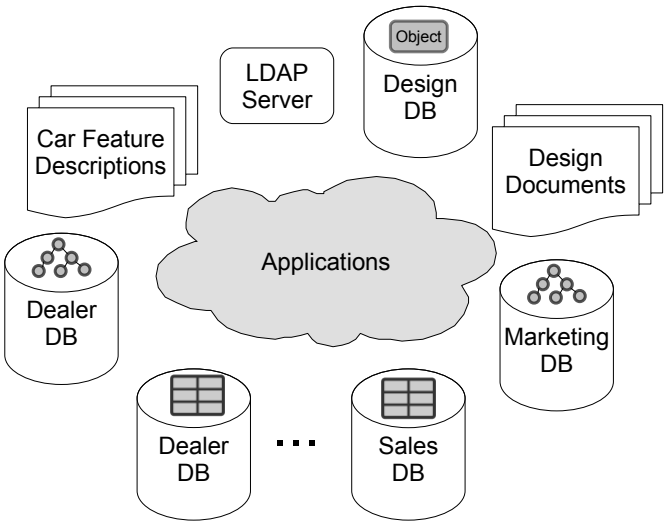


Figure 1.1: The data in an automobile company

The customer data is spread through the databases in the dealers, the sales department and the service department. Prospective customer data, which is not as reliable as the data for existing customers, is maintained in the marketing department. The car design data is in an object-oriented database and the manufacture data is in a relational database. The design documents are managed by a content management system in ODF or Docbook format (both are standards for representing documents in XML). The car feature descriptions, which need to be exchanged with dealers, are maintained in an XML repository. A part of the employee data is in the LDAP server, while other parts are in a database in the human resource department.

Suppose that an application assisting car sales needs to collect data about the customers, employees, sales, car designs and features. A number of problems make it hard to develop such kind of applications:

- the data is distributed into different locations: it is scattered across different departments and dealers.
- the data is heterogeneous: it is in different models such as relational models, object-oriented models, XML data models and even the hierarchical LDAP data models.
- the data is autonomous: it is managed by independent information systems, defined by different schemas.

- the data is sensitive: some data contains private information of employees or customers; some data is confidential information for the company; some data is business secrets between the company and its dealers.
- the data is in various qualities: some data, such as the employee data, is in high quality; some data, such as the customer data, contains lots of errors due to inaccurate data entry (the customer data in the marketing department) or the evolution of the databases (the customer data in the dealers).

If this application is built directly, it has to be adapted to different data models and information systems, various data qualities and diversified security mechanisms. Even worse, there could be a large number of applications which rely on the data and for each one these adaptation steps need to be repeated. It is vastly desirable to prepare the data in a general, uniform framework before feeding them into such applications. □

The complex nature of the real-word data means that no single technology can resolve all the problems associated with them. Different technologies need to be utilized to improve different aspects of the data. These aspects are classified into three categories and the techniques used to improve them are discussed below.

1.1.1 Real world data needs to be cleaned

Dirty data is everywhere. Do you have experience of receiving letters addressed to people who moved out long ago? Such a mistake is caused by dirty data. A recent survey [Red98] reveals that enterprises typically expect data error rates of approximately 1%–5%. The consequences caused by dirty data may be severe. It has been estimated that poor quality customer data costs U.S. businesses $611 billion annually in postage, printing and staff overhead (cf. [Eck02]). The process of detecting and removing errors and inconsistencies from the data in order to improve its quality is referred to as *data cleaning* [RD00].

The data quality problem may arise in any information system, particularly in those systems where the integrity constraints can not be or have not been enforced. In fact, even in databases with well defined integrity constraints, errors are still common. In a widely used, comprehensive taxonomy of dirty data [KCH$^+$03], wrong data which can not be prevented by traditional integrity constraints present a large category of dirty data. However, most existing constraint-based data cleaning research is based on traditional dependencies

(e.g. functional, full dependencies, etc.), which were developed mainly for schema design. Constraints combining traditional dependencies and the features for data cleaning tasks are essential to improve the quality of data.

Even worse, the data quality problem becomes more evident in applications such as data integration, data warehousing and data mining: errors could be propagated and exemplified in these systems and lead to useless, or even harmful results. This explains why data cleaning has been playing an increasingly important role in data warehousing and data mining projects. It is reported that 41% of data warehousing projects fail mainly due to data quality problems [Gro99]. Data cleaning has been regarded as a crucial first step in Knowledge Discovery in Databases (KDD) process [HS98].

Thus, a key technique to improve the usability of the data is data cleaning. It is estimated that the labour-intensive and complex process of data cleaning accounts for 30%-80% of the development time in a typical data warehouse project (cf. [ST98]). How to ultimately automate this labour-intensive process to effectively and efficiently clean relational data is the first problem to be investigated in the thesis.

1.1.2 The cleaned data needs to be integrated

With the advance of hardware and software technologies, more and more information systems are deployed at the departmental level and on desktop PCs, which are interconnected by modern network facilities. The data to be shared between these systems has been growing very fast, either inside an organization or between organizations. This data is not only distributed, but also heterogeneous. Different information systems have different schemas and possibly different data models. Furthermore, different applications have different interfaces and data formats. Most of the information needs to be exchanged in electronic formats. However, the exchange of data in their original model and format incurs numerous efforts to translate and integrate data among the data sources.

The wide adoption of XML as a standard for exchanging data has greatly reduced the efforts needed for data exchange: each system converts its data into XML format and subsequently all the data is exchanged in XML documents. The development of an efficient XML data exchange system calls for both a general mechanism to transform the data in other models to XML formats and a formalism to integrate distributed, autonomous XML

data into a single XML document.

The former, often referred to as *XML publishing*, has been investigated for several years. A number of prototype systems for XML publishing, for instance, SilkRoute [FTS00], XPERANTO [CKS+00] and PRATA+ [CFJK04] have been built with great success. Moreover, most mainstream database management systems have provided XML publishing functionalities.

The latter, referred to as *XML integration*, however, has not attracted as much research as XML publishing. In contrast with data integration in the relational context, new requirements have been imposed to XML data integration. First, both the source data and the integrated data are in XML model. Second, an integrated view always needs to be materialized in order to be sent to other parties. Third and most importantly, the integrated XML document is usually required to conform to an existing public schema defined by a standard, a community or an application. Last, building a system to efficiently integrate distributed data into a complex XML document requires not only a flexible framework but also sophisticated optimization techniques. Although several XML data integration systems exist, none of them addresses all of the above issues. XML data integration is the focus of the second part of the thesis.

1.1.3 The integrated data needs to be protected

The data exchanged between applications often contains sensitive information such as business secrets. Any unintended disclosure of the information would cause severe problems. The success of any information system does not only depend on the quality and the integration of the data, but also relies on the effective protection of this valuable, yet sensitive data. The security problem appears throughout the life cycle of the data, from its generation, storage, manipulation, to its integration, exchange and disposal. Lots of techniques exist for securing data in some of these processes. For example, most of the source data could be protected by the security mechanisms built into the source systems, such as DBMS or OS; the transmission of the data through network could be protected by secure network protocols... However, no matured technologies exist to secure the integrated XML data.

The protection of the integrated data calls for a generic, flexible security model that can effectively control access to XML data at various levels of granularity. The access control

in relational databases is driven by views: security administrators specify views for each user group; subsequently, any user is allowed to access the data only through a view over it. It is natural to extend this view mechanism into XML data management.

Even more importantly, enforcing such access control models should not imply any drastic degradation in either performance or functionality for the underlying XML query engine. In this sense these views need to be kept virtual because the number of views to be materialized could be prohibitively large due to the large number of user groups. Although relational views are widely available in all mainstream database systems, no virtual XML views are supported by any XML data management system, particularly when the views are recursively defined. In the last part of the thesis, the query rewriting and evaluation techniques are developed to support the enforcement of XML access control through virtual views. Given the ubiquitous of XML in modern information systems, this virtue view mechanism is not only critical to access control, but also increasingly demanded in other XML related contexts.

1.2 The CLINSE Framework for Cleaning, Integrating and Securing Data

In order to make effective and efficient use of the dirty, distributed and sensitive data, novel formalisms, algorithms and techniques are called for to clean, integrate and secure this data. This thesis addresses the challenges classified above in an integral framework, called CLINSE (CLeaning, INtegrating and SEcuring data), which makes use of both relational and XML data management techniques.

As shown in Figure 1.2, CLINSE framework has three parts. The relational data is first processed by the *data cleaning sub-framework* to improve its quality. Then, the cleaned relational data and the data in other non-XML sources are published into XML format. Subsequently, the *XML integration sub-framework* extracts data from all the sources and constructs a single XML document. At last, the *XML security sub-framework* ensures that users can access the integrated XML data only through an authorized view in order to protect the sensitive information. The models, methods and algorithms in these sub-frameworks are introduced below.

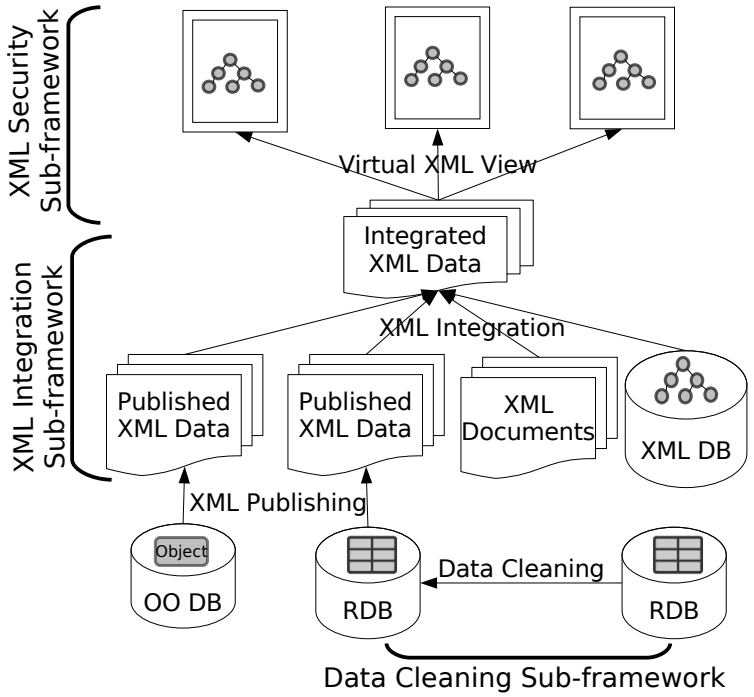


Figure 1.2: CLINSE framework to clean, integrate and secure data

1.2.1 Clean data with Conditional Functional Dependencies

Dirty data in a database often emerges as violations of integrity constraints. As a result, constraint-based technique is an important approach to clean data. In a constraint-based data cleaning approach, the core is a set of constraints which are defined to model the correctness of the data. Subsequently, potential errors are characterized as the *inconsistencies* in the data with respect to those constraints. The quality of the data is improved by *detecting* these inconsistencies and *repairing* them to restore the database to a consistent state.

Few work [BFFR05, LB07b] on constraint-based data cleaning has been reported and all of them use traditional database integrity constraints, such as functional dependencies, inclusion dependencies or denial dependencies, to model the quality of data. Whereas, in practice, these constraints are often not sufficient to improve the data quality. One reason is that traditional integrity constraints are always supposed to hold on the whole database. In a data cleaning context, due to schema evolution or data integration, it is common that the constraints only hold for a subset of the data. This motivate us to bring conditions into

constraints.

Moreover, in a data cleaning system based on traditional constraints, when the number of constraints grows large, the efficiency of maintaining these constraints and using them to detect and repair dirty data becomes a problem. This is because the traditional constraints are not designed for the context where a large number of constraints need to be specified. However, in data cleaning, sometimes lots of constraints are needed to capture the errors in data. One example is that, to discover dirty address data, a data cleaning system often needs to specify the constraints between the addresses and all the postal codes for a country or several countries which could be larger than the data instance itself. Thus, a type of constraints designed for data quality should also allow efficient processings in data cleaning.

In light of these requirements, CLINSE framework employs a novel extension of Functional Dependencies (FDs), referred to as Conditional Functional Dependencies (CFDs), to capture the consistencies of data. Unlike FDs which were developed mainly for schema design, CFDs are particularly proposed for the detection and repair of dirty data by extending FDs to allow bindings of semantically related values. CFDs are conditional because the data bindings, if present, restrict the dependencies applying only to a subset of the relations. This extension greatly increases the flexibility of the constraints: in situations where FDs do not hold, CFDs can be defined to detect inconsistencies; even in the case where FDs do hold, CFDs can still catch more errors in data than FDs because the bound values carry more information about the semantics of the correct data. This flexibility is critical for improving the quality of data — the capability of a data cleaning system is always limited by the range of errors it is able to discover in the data.

Based on the CFDs model, an efficient method to detect inconsistencies is developed in CLINSE framework. The detection is done by standard SQL queries, the size of which only increases with the embedded FDs and is independent of the bound data values. The pure SQL nature of the queries makes it possible to take full advantages of database index and optimisation techniques, which lead to very efficient inconsistencies detections. One may think that the additional flexibility of CFDs will decrease the performance of the detection, compared with FDs. However, this is, surprisingly, not true — the bound data values, when they are present, actually help detect inconsistencies more quickly. Additionally, incremental detection techniques are developed in CLINSE: when the database is updated,

minimum work is needed to re-detect the inconsistencies.

Better still, the additional information of the correct data carried by the data bindings provides more semantic information for repairing an inconsistent database. In fact, the data binding could be seen as a general way to model domain knowledge in a data cleaning framework. One advantage of modelling domain knowledge this way is its scalability: it is treated as ordinary data tables in the database and its size is only limited by the capability of the database system. CFDs provide a solid foundation for the automated repair and incremental repair modules of the CLINSE framework.

As shown in [BFFR05], the problem of finding a quality repair is NP-complete even for a fixed set of traditional FDs. This problem remains intractable for CFDs, and that FD-based repairing algorithms may not even terminate when applied to CFDs. To this end the cost model of [BFFR05] that incorporates both the accuracy of the data and edit distance is adopted in CLINSE. Based on the cost model, The FD-based repairing heuristic introduced in [BFFR05] is extended such that it is guaranteed to terminate and find quality repairs when working on CFDs.

The problem for incrementally finding quality repairs does not make our lives easier: it is also NP-complete. In light of this an efficient heuristic algorithm is developed for finding repairs in response to updates, namely, deletions or insertions of a group of tuples. This algorithm can also be used to find repairs of a dirty database.

The accuracy and scalability of these methods are evaluated with real data scraped from the Web. The experiments shows that CFDs are able to catch inconsistencies that traditional FDs fail to detect, and that the repairing and incremental repairing algorithms efficiently find accurate candidate repairs for large datasets.

CFDs and the proposed algorithms are a promising tool for cleaning real-world data. The algorithms developed in CLINSE are the first automated methods for finding repairs and incrementally finding repairs based on conditional constraints.

1.2.2 Integrate data with XML Integration Grammars

An important new requirement for extending data integration from relational context to XML context is the schema conformance. In relational databases, the schema is private to the data management systems. Whereas, in XML data management, the schema is often

public and a large number of XML schemas are even standards. Consequently, the global schema in XML data integration should be an input to the data integration system, rather than being defined in the data integration process. No existing system which integrates data from XML sources takes into account this requirement.

In CLINSE framework, a novel formalism, *XML Integration Grammars (XIGs)*, is proposed for specifying DTD-directed integration of XML data. Abstractly, an XIG maps data from multiple XML sources to a target XML document that conforms to a predefined DTD. An XIG extracts source XML data via queries expressed in a fragment of XQuery, and controls target document generation with tree-valued attributes and the target DTD. The novelty of XIGs consists in not only their automatic support for DTD-conformance but also in their *composability*: an XIG may embed local and remote XIGs in its definition, and invoke these XIGs during its evaluation. This yields an important modularity property for the XIGs that allows one to divide a complex integration task into manageable sub-tasks and conquer each of them separately.

Based on the XIG formalism, a sub-framework for DTD-directed XML integration, including algorithms for efficiently evaluating XIGs, is developed in CLINSE. How to capture recursive DTDs and recursive XIGs in a uniform framework is demonstrated, and a cost-based algorithm for scheduling local XIGs/XML queries and remote XIGs to maximize parallelism is proposed. An algorithm for merging multiple XQuery expressions into a single query without using "outer-union/outer-join" is provided. Combined with possible optimization techniques for the XQuery fragment used in XIG definitions, such optimizations can yield efficient evaluation strategies for DTD-directed XML integration.

1.2.3 Secure data with XML security views

To protect the sensitive integrated XML data, CLINSE adopts a view based security model proposed in [FCG04]: (1) the security administrator specifies an access policy for each user group by annotating the DTDs of an XML document; (2) a derivation module automatically derives the definition of a security view for each user group which consists of all and only the accessible information with respect to the policy specified for that group; (3) meanwhile, a view schema characterizing the accessible data of the group is also derived and provided to authorized users so that they can formulate their queries over the view.

This view based security model provides both schema availability, namely, view DTDs to facilitate authorized users to formulate their queries, and access control, i.e., protection of sensitive information from improper disclosure.

A central problem in a view based security framework is how to answer queries posed on the views. One way to do this is first materializing the views and then directly evaluating queries on the views. However, in XML security context, there are often a large number of users for the same XML document, which lead to lots of user groups and views for those groups. It is prohibitively expensive to materialize and maintain so many views. A realistic approach is to *rewrite* (aka. translate, reformulate) queries on the views into equivalent queries on the source, evaluate the rewritten queries on the source *without materializing the views*, and return the answers to the users. This is the approach used in CLINSE.

Although there has been a host of work on answering queries posed on XML views over relational data, little work has been done on querying virtual XML views over XML data, where query rewriting has only been studied for non-recursive XML views, over which XPath rewriting is always possible [FCG04]. Query rewriting for *recursive* views over XML is still an *open* problem [KCKN04].

In CLINSE framework, the problem of answering queries posed on possibly recursive views of XML documents is studied and efficient solutions are provided. It is shown that XPath is *not* closed under query rewriting for *recursive* views. In light of this CLINSE uses a mild extension of XPath, *regular XPath* [Mar04b], which uses the general Kleene closure E^* instead of the '//' axis. This regular XPath is *closed* under rewriting for arbitrary views, recursive or not. Since regular XPath subsumes XPath, any XPath queries on views can be rewritten to equivalent regular XPath queries on the source.

However, the rewriting problem is *EXPTIME-complete*: for a (regular) XPath query Q over even a non-recursive view, the rewritten regular XPath query on the source may be inherently *exponential in the size of Q and the view DTD D_V*. This tells us that rewriting is beyond reach in practice if Q is *directly* rewritten into regular XPath.

To avoid this prohibitive cost, CLINSE uses a new form of automata, *mixed finite state automata* (MFA) to represent rewritten regular XPath queries. An MFA is a nondeterministic finite automaton (NFA) *"annotated"* with alternating finite state automata (AFA), which characterize data-selection paths and filters of a regular XPath query Q, respectively. The algorithm rewrites Q into an equivalent MFA $\mathcal{M}$. In contrast to the exponential

blowup, the size of $\mathcal{M}$ is bounded by $O(|Q||\sigma||D_V|)$. This makes it possible to efficiently answer queries on views via rewriting. To our knowledge, although a number of automaton formalisms were proposed for XPath and XML stream (e.g. [DFFT02, GGM$^+$04]), they cannot characterize regular XPath queries, as opposed to MFA.

In CLINSE, an efficient algorithm, called HyPE, is provided for evaluating MFA $\mathcal{M}$ (rewritten regular XPath queries) on XML source T. While there have been a number of evaluation algorithms developed for XPath, none is capable of processing automaton represented regular XPath queries. Previous algorithms for XPath (e.g., [Koc03]) require at least two passes of T: a bottom-up traversal of T to evaluate filters, followed by a top-down pass of T to select nodes in the query answer. In contrast, HyPE combines the two passes into a single top-down pass of T during which it both evaluates filters and identifies potential answer nodes. The key idea is to use an auxiliary graph, often far smaller than T, to store potential answer nodes. Then, a single traversal of the graph suffices to find the actual answer nodes. The algorithm effectively avoids unnecessary processing of subtrees of T that do not contribute to the query answer. It is not only an efficient algorithm for evaluating regular XPath queries (MFA), but also an alternative algorithm to evaluate XPath queries.

A novel indexing technique to optimize the evaluation of regular XPath queries is also developed in CLINSE. While several labeling and indexing techniques were developed for evaluating '//' in XPath (e.g., [LM01, KMS02, SHYY05]), they are not very helpful when computing the general Kleene closure E^*, where E is itself a regular XPath query which may also contain a sub-query E_1^*. In contrast to previous labeling techniques, the indexing structure in CLINSE summarizes, at each node, information about its descendants of all different types in the document DTD. The indexing structure is effective in preventing unnecessary traversal of subtrees during FA (regular XPath) evaluation. This technique is in fact applicable to processing of XML queries beyond regular XPath.

The security sub-framework *fully* supports the rewriting and evaluation techniques mentioned above. An experimental study conducted on the system clearly demonstrates that the HyPE evaluation techniques are efficient and scale well. For regular XPath queries, HyPE evaluation of queries is compared with that of their XQuery translation, and it is found that the latter requires considerably more time. Furthermore, HyPE outperforms the widely used XPath engine Xalan (default XPath implementation in Java 5), whether Xalan uses its in-

terpretive processor or its high performance compiling processor (XSLTC), when evaluating XPath queries.

In summary, the security sub-framework of CLINSE does not only provide effective and efficient access control layer for the integrated XML data, but also contain the first practical and complete solution for answering regular XPath queries posed on (virtual and possibly recursively defined) XML views. It is provably efficient: it has a *linear-time* data complexity and a quadratic combined complexity. Furthermore it yields the first efficient technique for processing regular XPath queries, whose need is evident since regular XPath is increasingly being used both as a stand-alone query language and as an intermediate language in query translation [FYL+05].

1.3 Outline of Dissertation

The remainder of this thesis is organized as follows.

Chapter 2 provides background about cleaning relational data. It introduces the basic methods of data cleaning and cites relevant work in these areas.

Chapter 3 formally defines CFDs, presents the SQL techniques for detecting and incrementally detecting CFD violations, followed by the experimental study. This work is taken from [BFG+07].

In Chapter 4, the algorithms for finding repairs and incrementally finding repairs are developed and experimental results are presented. This work is taken from [CFG+07].

Chapter 5 explains how to publish the repaired relational data to XML format and provides background about XML data management.

Chapter 6 defines XIGs, followed by XIG examples, presents an XIG-based framework for XML integration. It provides algorithms for evaluating XIGs, followed by experimental results. This work is taken from [FGXJ04].

Chapter 7 discusses the closure property of (regular) XPath rewriting. Then, it introduces MFA and describes the rewriting algorithm. It also presents the MFA evaluation and optimization algorithms, followed by experimental results. This work is taken from [FGJK07] and [FGJK06].

Chapter 8 concludes the thesis.

Chapter 2

Cleaning Relational Data: Background and the State of the Art

Although a few special data cleaning problems, for example, data merge/purge (*a.k.a.*, record linkage), have been studied for a long time, data cleaning in general is relatively new compared with other established areas such as data integration and data mining which have been widely investigated for more than a decade. The theories, models, algorithms and systems for data cleaning are still in their early stages. However, the importance of data cleaning has been increasingly recognized as more and more data warehousing and data mining systems fail due to poor quality of data.

There are a lot of problems associated with data cleaning. What is dirty data? How to model and discover errors in data? Which kind of dirty data could be repaired and how to repair it? How to incorporate domain knowledge to assist data cleaning? How to build a data cleaning system? Will the results of a fully automatic data cleaning method be satisfiable? How to combine and trade-off human interactions in a semi-automatic data cleaning framework? Some of these problems have been addressed in prior work.

2.1 Dirty data versus clean data: how to define it

The errors in data arise with various reasons:

- The data in an organization is often accumulated within a long period of time measured by years or even decades. The schemas and constraints changed time by time

in their history.

- No integrity constraints are defined on the data or the integrity is enforced in the applications which are bypassed when the database is directly accessed.
- There are errors in data entry which can not be detected by integrity constraints.
- The data is mis-translated when it is integrated from different sources...

In [KCH+03], a comprehensive classification of dirty data is developed. In that taxonomy, the dirty data is classified hierarchically, with missing data, wrong data and unusable data at the top level. The wrong data are further divided into wrong data due to non-enforcement of enforceable constraints and that due to non-enforceability of constraints. Although this taxonomy is very helpful for understanding the sources and forms of dirty data, by no means it can serve as a definition of dirty data.

Interestingly, although a host of work has studied the concepts in data quality, there is no widely accepted formal definition of clean data and dirty data. Early literature [Kri79, BP85] uses correctness to define data quality. For instance, [BP85] regards the data in which the recorded value is in conformity with the actual value as clean. However, the clean data in one user's eyes could be dirty in others' eyes. Indeed, the correctness of data, depends on its context and purpose. For example, an address value with only a mail box could be regarded as correct in one application where postal address is required, while incorrect in another application where home address is desired. It is hard, if possible, to give a sound and complete formal definition for "error" or "dirty data" that is independent of its context — all existing definitions are descriptive and contain only some types of errors. Most recent work [Orr98, Wan98] adopts the concept of "fitness for use": clean data is defined as data that is fit for use by data consumers [WS96, SLW97]. This results in a context dependent, multidimensional concept of clean and dirty data.

A lot of dimensions are used in data quality literature to define the dirtiness of data. For example, [WS96] presents a survey of 179 dimensions suggested by various data consumers. Accuracy, consistency, relevancy, completeness and timeliness are the most frequently found dimensions in literature. A piece of data is *accurate* if it correctly represents the real world value. It is *consistent* if there are no conflicts in it. It is *relevant* if the data and its granularity are of interest. It is *complete* if all needed information is included and it is *timely* if it is up to date. Although each of the dimensions captures one aspect

of potential dirty data, these multidimensional definitions can not be used directly in data cleaning.

2.2 The dirty data to be cleaned: how to model it

Since the definition of the dirty data is multi-dimensional, it would be natural to ask: which dimensions are considered in data cleaning? In other words, what type of errors could be cleaned?

At first glance, it seems that any dirty data can be detected and repaired, at worst, by manually inspecting each value in the database by a domain expert. This is, however, not true even if such a labour intensive process is affordable — some data is simply not verifiable if no related information exists in the source or anywhere else. For example, a transaction record of a customer's shopping long time ago can not be verified if the customer can not remember it and the log for this transaction in the store has been deleted. Errors in data could be discovered and corrected only if there is sufficient information for that piece of data from the same database, external sources, or both. For manual data cleaning, these external sources could be the ones who input the data, or domain experts in the application area. In automatic data cleaning, these external sources would be the domain knowledge built into the data cleaning model.

Manual data cleaning is usually not affordable: it is laborious and time consuming. Moreover, it is subjective and sometimes leads to bad repair. A widespread misunderstanding is that manual repair always achieves better quality than automatic one. In practice, it is not uncommon to get bad manual repair because of the insufficient information a domain expert is aware of or make use of. In many cases it is not feasible for a domain expert to retrieve and inspect all the relevant information required to produce a good repair, even with the aids of some tools. Worse still, the expert will not know whether their repair will be consistent or not with other data in the database until the repair is applied.

In (semi-)automatic data cleaning, instead of using the multidimensional concept of dirty data, errors are defined within the scope of a model capturing the quality of data. Therefore, in order to find out what type of errors could be cleaned, another related question has to be answered: how do we model the data for the purpose of cleaning it?

The most widely used models for data cleaning are *rule-based models*. The idea of

using rules to improve data quality has long been practiced in data processing systems. In many web applications, the user inputs are verified against a set of *validation rules* encoded in scripting languages such as Java script to reduce the errors in data entry. In database systems, *integrity constraints*, such as keys, foreign keys, are employed to prevent undesired data from damaging the state of a database.

Different types of rules have been used for data cleaning. These rules are used to characterize either clean or dirty data:

Constraints In relational databases, integrity constraints are used to ensure that no change would be allowed if it destroys the consistency of data by enforcing predicates on relations. These predicates have to be satisfied to correctly reflect the real world. In general, an integrity constraint can be an arbitrary sentence from first-order logic pertaining to the database. However, arbitrary predicates may be costly to test [SKS01c]. Functional dependencies and inclusion dependencies are examples of common integrity constraints found in database practice. In *constraint-based data cleaning*, a set of constraints is defined to capture the semantics of clean data; subsequently, a piece of data is inconsistent (containing errors) if it *violates* the constraints defined in the model. These detected errors are then repaired to make the data consistent. In other words, the errors detected and repaired in constraint-based models are *inconsistencies* in the data with respect to the constraints.

Association Rules [HGG01] proposes error detection techniques based on association rules. Given sets of items X, Y in a collection of transactions, an association rule is of the form $X \rightarrow Y$ which indicates that whenever a transaction contains all items in X then it is likely to also contains all items in Y with a probability called *rule confidence*. The basic idea for *association-rule-based data cleaning* is first generating association rules from the training data and then applying them to the evaluating data. Usually the training data and evaluating data are originated from the same data set. For each record in the data, some of these rules may be supported, some rules may not be applicable to it, one or more rules may contradict with it. Finally a score is computed for every record as the number of violated rules weighted by their confidences. The records with high scores are suggested as potential errors. The hypothesis behind this model is that the generated association rules capture the nor-

mality of the considered data. This is consistent with constraints: both of them are used to characterize the regularities of clean data. The difference is that association rules are mined from the data and the violations might not be errors sometimes. By contrast, although nothing prevents constraints to be discovered from data, they are usually composed by domain experts and a violation always suggest an error in the conflicting data.

Edit Rules In data editing, an *edit* is a restriction to a single field in a record to ascertain whether its value is valid, or to a combination of fields in a record to ascertain whether the fields are consistent with one another. Here a record is a set of recorded answers to all the questions on the questionnaire [FH76]. For example, in a single-field edit we might want the number of children to be less than 20; in a multi-field edit we might want an individual of less than 15 years to always have marital status of unmarried. Data editing is the activity to detect and correct errors (logical inconsistencies) in data, especially in survey data.

Cleansing Rules In practice, data cleaning is often conducted by a set of cleansing rules. Each cleansing rule consists of two parts: a *condition* and an *action* which is triggered when the condition is satisfied. The action could be simply reporting the error detected, removing that record or repairing the involved values[Rit06]. An example of cleansing rule is that whenever the value 1 occurs in the Gender field whose domain is M and F (condition), the value needs to be changed to F (action). Cleansing rules are different from the above types of rules due to the fact that each rule has an explicit action defined in it while none of the above types of rules have. This is a procedural way to clean data, as contrast to the declarative means of the above three types of rules. Cleansing rules are analogous to triggers in database systems. However, triggers are activated by the change of the state of a database; cleansing rules are executed by users of a data cleaning system.

Of course, the above classification by no means reflects the theoretical properties of the rules used in data cleaning and there are lots of overlaps between these categories. For example, edits could be expressed as constraints in a form of logic and constraints can be used as the conditions in cleansing rules. The purpose of this classification is to show

different views on data cleaning from different communities: database (constraints), data mining (association rules), statistical research (edits) and industry (cleansing rules). In particular, a lot of work has been done in the areas of constraint-based data cleaning and statistical data editing. In the next two sections, we will review the research in those two areas.

Most previous research on data cleaning falls into the above rule-based models. There are a few exceptions, including the work using probabilistic models, clusters or patterns to model the regularities in data. In these models, no explicit rules are discovered from data or composed by domain experts. These models are discussed in Section 2.5.

This model based definition has a direct effect: an error in one model could be clean data in the other model. From this point of view, no data cleaning framework is complete — each framework can only find and fix the type of errors it models. The relative definition also makes it difficult to compare different data cleaning methods due to the lack of a consensus on the dirtiness of a value.

2.3 Constraint-based data cleaning

From the data cleaning point of view, there are three levels of dirty data:

1. the data in a database that is dirty according to the multidimensional concept of fitness for use;

2. the dirty data that could be captured by the current model; and

3. the dirty data that could be captured by the model without additional information beyond the database itself.

The first type of dirty data includes the second type and, in addition, it contains the dirty data that can not be captured by the current model. Similarly, the second type of dirty data includes the third type and it also contains the dirty data that could be captured with additional domain knowledge. The range of dirty data a constraint-based system can deal with is limited by its ability to enlarge the last two types of dirty data. Although lots of dimensions are included in the first type of dirty data, only the consistency dimension is

captured by constraint-based models. Thus, one principle of constraint based data cleaning is to *maximize the dirty data characterized by the consistency dimension*.

As long as dirty data in a database is captured as inconsistencies with respect to a set of integrity constraints, a clean database, called a *repair*, could be computed to resolve these inconsistencies. The concept of database repair is introduced in [ABC99], where a repair is used as an auxiliary notion for defining *consistent query answering*, which will be discussed in Section 2.3.3. Obviously, in constraint-based data cleaning, a repair must satisfy all constraints defined in the model, but there could be lots of such repairs for the same database. For example, a repair can be obtained by simply remove all of the inconsistent tuples repeatedly until a consistent database is obtained (this process needs to be repeated when inclusion dependencies are presented). Therefore, the system should distinguish good repairs from bad ones by certain computable measures. Following this principle, a database repair is defined as follows:

A constraint-based data cleaning model consists a relational database D to be cleaned and a set C of constraints defined on D to characterize the semantics of the data. Database D is **dirty** if it is inconsistent under constraints C, i.e. $D \not\models C$. A **repair** of the dirty database D is specified as a consistent database D' derived from D such that $D' \models C$ and D' *minimally differs* from D.

Constraint-based data cleaning differs from one to another due to different choices of minimization measures, classes of constraints, repair operations used in the model and weather it is query-oriented or repair-oriented. Normally, data cleaning is *repair-oriented*, in other words, the result of data cleaning is to get a repaired database which is materialized. An opposite approach is *query-oriented* data cleaning where the dirty database will remain to be inconsistent, but it presents the users who query this inconsistent database with consistent answers. This virtual repair approach is referred to as *consistent query answering* in literature.

2.3.1 Constraints.

As presented earlier, a repair must satisfy all the constraints defined in the model. Using different classes of constraints will lead to different repairs. The major constraints used previously in data cleaning include denial constraints, full dependencies, functional dependen-

cies and inclusion dependencies. In the following we briefly review these constraints. The work using them is presented in section 2.3.3 and 2.3.4. We assume a relational database schema $\mathcal{R}$ is a collection of relation symbols $(R_1, \ldots, R_n)$. An atomic formula is either of the form $R_i(\bar{x}_i)$, where $1 \leqslant i \leqslant n$ and R_i is a d-ary relational symbol, or else a built-in predicate. Here $\bar{x}_i$ is a tuple of variables and constants. The variables in tuples $\bar{x}_1, \ldots, \bar{x}_m$ are denoted by $x_1, \ldots, x_k$. A special build-in predicate of the form $x_i = x_j$ is called *equality*, where x_i and x_j are individual variables.

Universal Integrity Constraints

$$\forall x_1, \ldots, x_k.[R_1(\bar{x}_1) \vee \cdots \vee R_s(\bar{x}_s) \vee \neg R_{s+1}(\bar{x}_{s+1}) \vee \cdots \vee \neg R_m(\bar{x}_m) \vee \phi(x_1, \ldots, x_k)]$$

where ϕ is a quantifier-free formula referring only to built-in predicates. It is called universal because no existential quantifiers are allowed in the constraints. A binary universal integrity constraint is a universal constraint where $m \leqslant 2$.

Denial Constraints

$$\forall x_1, \ldots, x_k.[\neg R_1(\bar{x}_1) \vee \cdots \vee \neg R_m(\bar{x}_m) \vee \phi(x_1, \ldots, x_k)]$$

Denial constraints are a special case of universal integrity constraints where relation symbols are only allowed in their negative forms.

Full Tuple-Generating Dependencies

$$\forall x_1, \ldots, x_k.[(R_1(\bar{x}_1) \wedge \cdots \wedge R_m(\bar{x}_m)) \rightarrow R_j(\bar{x}_j)]$$

where $1 \leqslant j \leqslant n$, $\bar{x}_1, \ldots, \bar{x}_m, \bar{x}_j$ are tuples of variables. In the next three classes of constraints, $\bar{x}_i$, $1 \leqslant i \leqslant m$ is always restricted to be a tuple of variables.

Full Equality-Generating Dependencies

$$\forall x_1, \ldots, x_k.[(R_1(\bar{x}_1) \wedge \cdots \wedge R_m(\bar{x}_m)) \rightarrow x_i = x_j]$$

where $1 \leqslant i, j \leqslant k$. They could also be written in a form closer to denial constraints:

$$\forall x_1, \ldots, x_k.[\neg R_1(\bar{x}_1) \vee \cdots \vee \neg R_m(\bar{x}_m) \vee x_i = x_j]$$

Full equality-generating dependencies are a special case of denial constraints: ϕ is limited to the form of $x_i = x_j$ and $\bar{x}_1, \ldots, \bar{x}_m$ is restricted to containing only tuples of variables (no constants are allowed any more).

Functional Dependencies

$$\forall \bar{x}_1, \bar{x}_2, \bar{x}_3, \bar{x}_4, \bar{x}_5. [(R(\bar{x}_1, \bar{x}_2, \bar{x}_3) \wedge R(\bar{x}_1, \bar{x}_4, \bar{x}_5)) \rightarrow \bar{x}_2 = \bar{x}_4]$$

Functional dependencies (FD) are a special case of full equality-generating dependencies where $m = 2$. An FD is often written as $R : X \rightarrow Y$ where X is the set of attributes of R corresponding to $\bar{x}_1$ and Y is the set of attributes of R corresponding to $\bar{x}_2$ and $\bar{x}_4$. A *key dependency* is an FD $R : X \rightarrow U$ where U is the full set of attributes of the relation R.

Inclusion Dependencies

$$\forall \bar{x}_1, \bar{x}_2, \exists \bar{x}_3. [R_1(\bar{x}_1, \bar{x}_2) \rightarrow R_2(\bar{x}_2, \bar{x}_3)]$$

An inclusion dependency (IND) is also referred to as a *referential constraint*. It is often written as $R_1[X] \subseteq R_2[Y]$ where X (resp. Y) is the set of attributes of R_1 (resp. R_2) corresponding to $\bar{x}_2$. If $R_2 : Y \rightarrow U$ is a key dependency, the inclusion dependency $R_1[X] \subseteq R_2[Y]$ becomes a *foreign key dependency*. An IND can be expressed by neither denial constraints, nor full dependencies. It is a special case of a tuple-generating dependency which is a more general form of full tuple-generating dependency.

2.3.2 Minimization measures.

Besides satisfying the constraints, another criteria for defining repair is that a repair should minimally differ from the original database. We refer the difference between a potential repair D' and the original database D as $\Delta(D', D)$. Using $\Delta(D', D)$, a partial order $\preceq_D$ between database instances $D'_1, \ldots, D'_k$ could be defined to model how close $D'_i, 1 \leqslant i \leqslant k$ is from D. Once this order is ready, a repair could be defined as the $\preceq_D$-minimal database instance D' among those D'_i such that $D'_i \models C$. Several measures have been employed for specifying $\Delta(D', D)$.

set difference

$$\Delta_{\text{set}}(D', D) = (D' \setminus D) \cup (D \setminus D')$$

where $D' \setminus D$ contains the tuples inserted during the repair process and $D \setminus D'$ contains tuples deleted. The assumption is that the database may be neither sound nor

complete. If the database is assumed to be inconsistent but complete, no tuple insertions need to be considered. In that case this *symmetric set difference* measure can be simplified as *asymmetric set difference*:

$$\Delta_{\text{aset}}(D', D) = (D \setminus D')$$

cardinality of set difference

$$\Delta_{\text{card}}(D', D) = |(D' \setminus D) \cup (D \setminus D')|$$

Instead of using the set difference itself, the cardinality of set difference can also be used to measure the difference.

number of value changes

$$\begin{aligned} \Delta_{\text{change}}(D'(t), D(t)) &= \sum_{A \in \text{attr}(R_i)} \text{diffcount}_{t,A} \\ \text{diffcount}_{t,A} &= \begin{cases} 1 & : \quad D'(t,A) \neq D(t,A) \\ 0 & : \quad D'(t,A) = D(t,A) \end{cases} \end{aligned}$$

where $\text{attr}(R_i)$ denotes the attributes of relation schema R_i. $\Delta(D', D)$ is defined by summing up $\Delta(D'(t), D(t))$ for all the tuples in each relation of the database.

weighted distance of values

$$\Delta_{\text{dis}}(D'(t), D(t)) = w_t \cdot \sum_{A \in \text{attr}(R_i)} w_A \cdot \mathsf{dis}(D'(t,A), D(t,A))$$

where $\mathsf{dis}(\cdot)$ is a distance function, w_t and w_A are weights optionally associated with tuple t and attribute A, respectively. Different distance functions and weights have been used in prior work. [BBFL05, LB07b] use L_1 and L_2 distances of numerical values and attribute weight. [BFFR05] uses edit distance of string values and tuple weight.

The set measure and numerical measure require different order $\preceq_D$:

set inclusion based partial order

$$D'_1 \preceq_D D'_2 \iff \Delta(D'_1, D) \subseteq \Delta(D'_2, D)$$

When $\Delta(D', D)$ is measured by set difference $(\Delta_{\text{set}}, \Delta_{\text{aset}})$, this order is used.

number comparison based total order

$$D'_1 \preceq_D D'_2 \iff \Delta(D'_1, D) \leqslant \Delta(D'_2, D)$$

All other measures defined above ($\Delta_{\text{card}}, \Delta_{\text{change}}, \Delta_{\text{dis}}$) use this order.

Different choices of $\Delta(D', D)$ lead to different repair semantics. For example, under asymmetric set difference minimization measure, a repair D' is a maximal subset of D such that $D' \models C$; while under cardinality of set difference measure, such a D' may not be a repair: there might be a D'_1, such that $D'_1 \models C$ and $\Delta_{\text{card}}(D'_1, D) < \Delta_{\text{card}}(D', D)$, i.e. $|\Delta_{\text{aset}}(D'_1, D)| < |\Delta_{\text{aset}}(D', D)|$ although $\Delta_{\text{aset}}(D'_1, D) \not\subset \Delta_{\text{aset}}(D', D)$. Under both measures, repairs need not be unique. The minimization measures have direct impact on repair operations. In the repairs defined by the first two measures ($\Delta_{\text{set}}, \Delta_{\text{card}}$), the minimal modification unit is usually a tuple. Furthermore, for asymmetric set difference based repairs, only tuple deletion is needed. Thus, the work using the first two measures often adopts *tuple-based* repair semantics. However, for the last two minimization measures ($\Delta_{\text{change}}, \Delta_{\text{dis}}$), tuple level repair operations are not enough to produce all repairs — attribute level repair operations are needed. Consequently, the data cleaning work using these minimization measures often takes value modification (tuple update) as its repair operation, which causes *attribute-based* repair semantics.

2.3.3 Query-oriented data cleaning: consistent query answering

Consistent query answering is one of the most investigated areas closely related to data cleaning. It is an approach to query inconsistent databases without explicitly repairing them first. Strictly speaking, consistent query answering is not data cleaning — the database is not physically cleaned, but kept to be inconsistent. On the other hand, consistent query answering overlaps with data cleaning — the database is virtually cleaned when user queries are answered. So the notion of repair is also needed in consistent query answering and the same concept is shared between both of them.

A consistent answer to a query over an inconsistent database is an answer that is invariant under all minimal restorations of consistency to the original database [ABC99]:

A tuple t is a consistent answer to a query Q over a database instance D with a set of constraints C if and only if t is an answer to the query Q over *every* repair D' of D with respect to constraints C.

In principle, to provide users with consistent query answers, the constraints need to be associated with either the inconsistent database or the user query. As a result, there are two flavors of consistent query answering: the *database patching strategy* (the constraints are associated with the database) or the *query transformation strategy* (the constraints are associated with the query).

Query Transformation Strategy. In the query transformation strategy, the inconsistent database is unchanged. Instead, the query Q is transformed into another form to incorporate the integrity constraints. In prior work, two types of the transformed form have been investigated. If the transformed form is in first-order, it can be easily formulated as an SQL query Q' and evaluated on any relational database system. This approach is referred to as *first-order rewriting*. Otherwise, the transformed form could be formulated as a disjunctive logic program P'. The final result is obtained by computing the stable models of the logic program P', i.e., the facts which are members of every answer set of P'. In both cases, the result obtained from the inconsistent database is equivalent to the intersection of the answers to the original query Q on all minimally repaired databases.

[ABC99, FM05] propose algorithms for consistent query answering under the symmetric set difference semantics by adopting first-order rewriting strategy. [ABC99] develops rewriting techniques for quantifier-free conjunctive queries in the presence of binary acyclic universal integrity constraints. In brief, query Q is expanded by new conditions to enforce the constraints C. These conditions, referred to as *residues*, are produced repeatedly by resolving literals in the possibly expanded query with constraints C. The process continues until no more changes occur. [FM05] proposes a rewriting algorithm for a large subset of conjunctive queries with existential quantification in the presence of primary key constraints. The subset is defined in terms of *join graph*: a directed graph with its vertices corresponding to the literals of the query and its arcs corresponding to each join in the query that involves some variables that are at the position of a non-key attribute. The algorithm runs in polynomial time in the size of the query. It works for conjunctive queries without repeated relation symbols whose join graph is a forest. [GLRR05] further gen-

eralize this technique to cope with exclusion dependencies. Two prototype systems using first-order query rewriting have been reported. [CB00] presents a system built on top of the XSB deductive database system [SSW94] following the method in [ABC99]. [FFM05] describes the ConQuer system based on the algorithms developed in [FM05].

The advantage of the first-order rewriting approach is that the construction of all repairs is entirely avoided. This is important especially for the set difference semantics which could potentially leads to large number of repairs. For example, in the worst case, exponential number of repairs may exists for a database with key dependencies [ABC$^+$03c]. Moreover, the rewritten query Q' can be expressed in SQL and therefore efficiently evaluated by any database management system without modification. Since the rewriting is not dependent on the database instance, it does not affect the data complexity of the overall consistent query answering. Thus, as long as query Q is first-order rewritable, we can always obtain a polynomial time (data complexity) solution for consistent query answering. However, only restricted classes of queries are first order rewritable. Even for constraints as limited as primary keys, [FM05] shows consistent query answering is *coNP*-complete for every query of a class whose join graph is not a forest and some conjunctive queries fall into that class. For larger constraints such as functional dependencies or denial constraints, existing first-order rewriting algorithms can only deal with quantifier-free conjunctive queries.

In light of the limitation of first-order query rewriting, techniques for query transformation based on logic programs have been developed. [ABC03b, GGZ03] capture all repairs of a database under the set difference semantics as answer sets of logic programs with negation and disjunction. Queries are then incorporated into these logic programs. In contrast to first-order rewriting scenario where relational database systems are used for evaluating Q', here consistent query answering has to be implemented using a disjunctive logic programming system such as DLV ([LPF$^+$06]). This approach can handle arbitrary universal constraints and first order queries. However, the problem of deciding whether an atom is a member of all answer sets of a disjunctive logic program is Π_2^p-complete [DEGV01]. Therefore, a direct implementation of consistent query answering using disjunctive logic programming systems is practical only for very small databases [Cho07].

Database Patching Strategy. In contrast to query transformation where the database instance is involved in cleaning process as late as possible, the database patching strategy is

an *eager approach*. The inconsistent database is amended by some auxiliary structures to incorporate the restrictions posed by the constraints. For instance, these auxiliary structures could be a compact representation of all possible repairs with respect to the constraints. Then the query is evaluated over the database and these auxiliary structures to get consistent answers.

[ABC01, ABC$^+$03c, CMS04, CM05, Wij05] follow the database patching strategy. [ABC01, ABC$^+$03c, CMS04, CM05] use *graph*, called conflict (hyper)graph to represent possible repairs, while [Wij05] uses *tableau*, called nucleus to help compute consistent answers. A *conflict graph* [ABC01, ABC$^+$03c] can represent all possible repairs under functional dependencies. It is an undirected graph with its vertices corresponding to the set of tuples in the database and each edge indicating two tuples connected by the edge have conflicts. Conflict graph is generalized as *conflict hypergraph* in [CMS04, CM05] to represent database repairs under denial constraints. The size of the conflict (hyper)graph is polynomial with respect to the number of tuples in the database instance. In conflict (hyper)graph, each repair corresponds to a maximal independent set. Based on this repair representation, polynomial algorithms have been proposed by [CMS04, CM05] to answer quantifier-free first-order queries with denial constraints under the asymmetric set difference semantics, and also by [ABC01, ABC$^+$03c] to answer group-by-free scalar aggregation queries such as min, max, count(*), sum and avg with at most one nontrivial functional dependency under the symmetric set difference semantics. A *nucleus* is a tableau where the attributes in a tuple can take not only constants but also variables as their values. [Wij05] shows quantifier-free conjunctive queries can be answered by nucleus in polynomial time with respect to key dependencies or contradiction-generating dependencies. A prototype system called Hippo has been built on top of PostgreSQL based on conflict hypergraphs [CMS04].

Similar as first-order query rewriting, these algorithms can not deal with unrestricted conjunctive queries efficiently. In fact, it has been shown that for conjunctive queries and constraints as restricted as primary key dependencies, consistent query answering is *coNP*-complete under the asymmetric set difference semantics [CM05] and under the symmetric set difference semantics [CLR03]. It is $P^{NP(log(n))}$-complete for ground atomic queries and denial constraints under the cardinality of set difference semantics [LB07a], while the same problem has polynomial time complexity under the set difference semantics [CM05]. More information on consistent query answering can be found in surveys [BC03, Ber06, Cho06,

Cho07].

2.3.4 Repair-oriented data cleaning: constraint repair

The repair-oriented data cleaning is also referred to as *constraint repair* [BFFR05] or *database fix* [LB07b]. In contrast with consistent query answering, little work has been published for repair-oriented data cleaning. The challenges and techniques are quite different between query and repair-oriented data cleaning although they share some common concepts.

Minimization Measure. The minimization measure in repair-oriented data cleaning is often more *selective* than that in query-oriented data cleaning. The reason is that in the latter no specific repair needs to be identified. It is not a problem if there are thousands of repairs for a single inconsistent database as long as consistent answers can be computed for user queries. But in the former, a specific repair needs to be singled out as the materialized fix to the inconsistent database. If there are too many legal repairs, the choice of the final fix could be arbitrary, which is not desired. For example, as we have seen before, the tuple based set difference semantics have been adopted by most of the work for consistent query answering. However, it is known that even in the presence of one functional dependency there may be exponentially many repairs. With only 80 tuples involved in conflicts, the number of repairs may exceed 10^{12} [ABC$^+$03c, CMS04]. The cardinality of set difference minimization measure is more selective than set difference measure: every repair in the former is also repair in the latter, but not necessarily the other way around. The most selective measures are *distance based measures* presented in 2.3.2. Consequently, most repair oriented data cleaning frameworks adopt attribute based semantics, particularly distance based minimization measures, in contrast to the prevalence of tuple based semantics in consistent query answering context.

Repair Operations. The selective minimization measure has effects on repair operations — it paves the way for fine-grained repair operations. We are not aware of any work in constraint repair adopts tuple deletion/insertion as repair operations which are popular in consistent query answering. Instead, *value modification* is used as the repair operation. Such fine-grained repair operation has the advantage of losing less information than those coarse-grained repair operations. In tuple-based repair, if a tuple is identified as dirty, all

values in the tuple are deleted. In fact, there might be only one dirty attribute. This whole tuple deletion causes the loss of all useful information in those clean attributes in the tuple. In contrast, when value modification is used to produce a repair, clean attributes are not affected by the repair operation. Moreover, the modification is guided by the minimization measure. The combined effects of the selective minimization measure and fine-grained repair operation are that the modified value would be as close as possible to the original value under the chosen distance measure. Thus the correct information in the original inconsistent database is maximally preserved, which is one of the primary goal of data cleaning.

[BFFR05] presents a heuristic algorithm for repairing inconsistencies based on standard functional dependencies and inclusion dependencies. The algorithm is based on merging equivalence classes. The minimization measure is the aggregation of edit distance of string values between the candidate repair and the original database with considerations of tuple weights. These weights are used to model the confidence on the original tuple. [LB07b] develops an efficient approximation algorithm to physically repair databases which is inconsistent in presence of denial constraints by updating numerical values. The minimization measure is L_1 distance (city distance) of numerical values with considerations of attribute weights. In both scenarios, the problem of determining if there is a repair at a distance smaller than a given value to the original database is *NP*-hard (in the former, it is shown to be *NP*-complete). [FPL$^+$01] uses disjunctive logic programming to repair census data which is inconsistent with respect to first-order logic. In contrast with [LB07b] and [BFFR05], the minimization measure is the number of value changes, which is independent of the corrected values. Obviously, there could be large amount of repairs under this measure. So another measure, the number of satisfied preference rules, is used to further restrict the minimal repairs. Like consistent query answering based on logic programs, the constraint repair system in [FPL$^+$01] is implemented on disjunctive logic programming system DLV ([LPF$^+$06]).

In summary, a number of techniques have been studied for consistent query answering and constraint repair. For the former, besides the computational complexity analysis, the focus has been identifying and finding efficient algorithms for tractable cases and proposing general solutions for intractable cases applicable to small data sets; for the latter, the focus has been developing approximation or heuristic algorithms to deal with the intractability.

Most of the work on consistent query answering adopts the tuple based semantics such as set difference or cardinality of set difference and deal with potentially huge number of repairs; while the work on constraint repair uses the attribute based semantics and allows only a few or even unique repairs.

2.4 Edit-based data cleaning: statistical data editing and imputation

Besides the work on constraint-based data cleaning conducted in the database research community, the problem of automatic correcting inconsistent values and filling missing values in survey data, which is referred to as *statistical data editing and imputation*, has long been investigated by statisticians. The solutions of the imputation problem are very close to constraint-based data cleaning in spirits.

The data quality problem has long been recognized by the statisticians. The large volume of census data may contain lots of errors and must be cleaned before any statistical analysis. This cleaning process consists of procedures to repair self-contradictory data and fill in missing data. Before 1950s, this work had been primarily done by manual review. Later the census data was often cleaned by a lot of if-then-else rules which are hard-wired in a program specifically built to clean the data. However, these tools are not reusable. Each time a new survey form is used, a new tool needs to be developed from scratch. To further reduce human efforts, statisticians make the if-then-else rules re-configurable by putting them in a database and reuse the data editing tool each time a new form is used — only the rules in the database need to be updated. Not surprisingly, this leads to similar models as constraints-based data cleaning.

The theoretical basis for a general data editing system, often called Fellegi-Holt model, is provided in [FH76]. Under Fellegi-Holt model, the data to be cleaned is a sequence of records. Each record contains a set of values which are encoded answers to a questionnaire. The inconsistencies in the data are captured as a subset of the total code space that is unacceptable. This subset is modeled by a set of rules, referred to as *edits*.

Data Edits. A statistical data collection could be defined in database terms as a relation. Each tuple t in the relation corresponds to a record. Each attribute A in the schema R of

the relation corresponds to a field (*a.k.a.* a variable) in the encoded questionnaire. More specifically, a *record schema* is a set of fields: $R = (A_1, \ldots, A_n)$ and a *record instance* is a set of values $t = (v_1, \ldots, v_n)$. Each field A_i takes either a numerical value that answers a question or a categorical value that encodes the answer to a question. For instance, $(8, 1, 2)$ is a record instance with schema $(\mathsf{Age}, \mathsf{Gender}, \mathsf{MaritalStatus})$. The record represents a person who is eight years old ($\mathsf{Age} = 8$), male ($\mathsf{Gender} = 1$, where 1 encodes "male", 2 encodes "female") and married ($\mathsf{MaritalStatus} = 2$, where 1 encodes "single", 2 encodes "married" and 3 encodes "divorced"). For convenience, from now on, we will write a record instance as un-encoded form such as $(8, \texttt{male}, \texttt{married})$. Obviously, there are errors in this record: an eight years old boy can not be married.

All valid values of A_i form the domain of A_i, referred to as $\mathsf{dom}(A_i)$. Each record takes values in the product space of these domains $\mathsf{dom}(A_1) \times \cdots \times \mathsf{dom}(A_n)$. This product space could be divided into two subset: the one that contains valid combination of values of a record and the other that contains invalid combination of values of a record. A *multi-field edit* is a rule to characterize the latter subset. It catches a record in which each vaule is valid itself, but their combination is invalid. An example multi-field edit to catch the above error is $e_1 = \{\texttt{age<15}, , \texttt{married}\}$ which indicates no matter what value the Gender field takes, being younger than 15 years old is incompatible with being married. A *single-field edit* is analogous to domain constraints in database systems. It specifies a record has an "out-of-domain" value. An example single-field edit is $e_2 = \{\texttt{age>150}, , \}$ which indicates the age of a person should not be larger than 150.

An edit is either a single-field edit or a multi-field edit. A set of edits E could be defined by domain experts for a collection of records. The edits serve the opposite purpose as constrains C in constraint-based data cleaning: edits express error condition, i.e. characterize dirty data, while constraints are used to model clean data. A record *failing* any edit in E is regarded as an inconsistent record and thus needs to be corrected. A consistent record is the one that *passes* (i.e., succeeds, or satisfies) all the edits.

Record Correction. An edit-based data cleaning model is defined as below:

An edit-based data cleaning model consists a collection of records D to be cleaned and a set E of edits to capture errors in D. A record t in D is **dirty** if it fails any edit in E. A **correction** of a dirty record t is specified as a consistent record t' derived from t such that (1) t' passes all edits in E; (2) fewest number of fields in t has been changed; and (3) the original joint frequency distributions of the data is preserved as far as possible. **Data editing and imputation** is the process of using edit rules to identify errors in records and find their corrections.

A correction for a collection of records is analogous to a repair in constraint-based data cleaning; the data editing and imputation is analogous to constraint repair. Similar to constraint-based data cleaning, the correction needs to satisfy all of the rules and respect the minimal change principle. Here, the minimization measure is the *number of values changed*. An additional requirement, which is not needed in constraint-based data cleaning, is the preservation of joint frequency distribution. This is needed to prevent the statistics of the data from being affected by the correction.

Error Detection. A merit of Fellegi-Holt model is that, in one pass through the data, for an edit-failing record, a minimal set of fields can be found. If these fields are changed it is guaranteed to yield a correction. The process of finding such a minimal set of fields is referred to as *error localization*. It is analogous to the error detection in constraint-based data cleaning. A difference is that in the latter only inconsistencies are detected, the erroneous values are not further identified among the inconsistent data. [FH76] has proven that one way to solve the error localization problem is to compute a *complete* set of edits — including both the edits explicitly specified by users and some implicit edits logically derived from the explicit ones. The process of deriving implicit edits is referred to as *edit generation* and the required implicit edits in error localization are referred to as *essentially new edits* in [FH76]. Although the guarantee of finding a correction by changing minimal set of fields is appealing, both edit generation and error localization are computationally intractable [GKL86]. To overcome these bottlenecks, a number of algorithms are proposed to speed up their computations. [GKL86, Win95, Win97, Che98] develop different alternatives of edit generation and error localization algorithms.

Edit Generation Unlike error localization which has to be computed in the cleaning process, edit generation could be precomputed because the record instance is not needed in the

computation. Some literature views edit generation as a pre-processing step for error localization [GKL86, Win95, Win97]. [GKL86] re-defines the complete set of edits in [FH76] as the original explicit edits plus the set of *maximal implicit edits*. By adopting maximal implicit edits, it removes the redundant edits which are not maximal, i.e. any edit that is properly included in another edit. It shows the re-defined complete edits are sufficient for solving the error localization problem and proposes an algorithm which is computationally superior to that of [FH76] for generating these edits. [Win95] observes that the edit generation algorithm in [GKL86] may fail in some situation and presents an alternative one, called EG algorithm, to correctly generates all maximal implicit edits. [Win97] uses a heuristic, called EGE algorithm, to reduce the computation at nonroot generating fields. It is much faster than EG algorithm and generates most of the implicit edits. [Che98] further improves the performance by only finding all prime cover solutions of the set covering problem which is needed in generating edits.

Edit Validation Another virtue of Fellegi-Holt model is that, prior to the receipt of data records, the mutual consistency of the explicit edits could be checked in the edit generation process. Thus, as a side effect, the edit generation also solves the *edit validation* problem which is in analogous to the consistency checking of constraints in a constraint-based data cleaning system.

Error Localization If the implicit edits are generated prior to editing, the amount of computation needed for error localization can be significantly reduced [Win99]. However, the generation of a complete set of edits often requires days-to-months of computation [Gar03, Win99]. Thus some approaches directly solve the error localization problem without computing implicit edits [San79, KMW88, dW96] or compute partial implicit edits on-the-fly [DW97]. However, In the latter, it is not guaranteed to find a solution for error localization. In the former, there is no control over how long it will take for a record. Those approaches usually introduce time-out mechanism to skip a record if it takes too much time. These records need to be manually inspected and corrected.

Relations to Logic. [BS01, BGH03] have shown the edits in Fellegi-Holt model could be expressed in propositional logic and the edit validation could be achieved by solving a sequence of Satisfiability problem, the edit generation is essentially the same as a technique for automating logical deduction called resolution.

The theories, algorithms developed for statistical editing and imputation problem have provided important solutions for rule-based data cleaning, in particular in the case where the set of rules are not large. In practical case, however, such methods suffer from severe computational limitations [Win99]. According to [Win99], it is unlikely that current algorithms can generate the full set of implicit edits with 300 explicit edits, while as many as 750 explicit edits may be needed by a large survey form or in complicated edit situations. In addition to this limitation on the size of the rules, the edits only express single-record (single-field or multiple-field) constraints that are commonly encountered in survey data. However, in a database context, the inconsistencies may arise due to relationship between tuples (functional dependencies) or between relations (inclusion dependencies). There is no efficient way to translate these constraints into small number of edits.

2.5 Beyond rule-based data cleaning

There are also work in which the dirty data is not captured by rules. One line of research is to identify errors as outliers and remove them. Another one is using data mining techniques to explain the data quality problem and suggest corrections of the errors — instead of removing them. In the first line of research, [Joh95] extends the pruning scheme in C4.5, a decision tree algorithm, to fully remove the effect of outliers. [AAR96] presents a linear algorithm to find deviations in large databases by simulating a mechanism familiar to human beings: after seeing a series of similar data, an element disturbing the series is considered as a possible error. A dissimilarity function is proposed to capture how dissimilar a new data item is from the data items seen so far. In the second line of research, [SW00] uses Bayesian techniques to detect and correct dirty data by taking advantage of dependencies between attributes and exploiting expert knowledge of the relationships among the attributes. [KM03] provides an algorithm for the unsupervised discovery of three probabilistic models: a generative model of the clean records, a generative model of the noise values, and a probabilistic model of the corruption process. These models are used to assist detecting and correcting dirty data. More methods are surveyed in [MM00].

In above approaches, whether the outliers or noises are errors or not depends on the domain. Sometimes, these outliers might be *correct* data that do not fit the clean model. Therefore, the correction of outliers should always be assisted by domain experts [LGJ03].

This non-deterministic nature limits their uses as independent automatic data cleaning tools. These methods are often used to assist semi-automatic cleaning of data.

2.6 Summary

In this chapter, the work on rule-based data cleaning is summarised. Most of the existing work is focusing on consistent query answering and statistical data editing and imputation problems. Little work has been done on constraint repair.

There are many scenarios where constraint repair is preferred than consistent query answering. In consistent query answering, most of the cleaning computations are pushed to query answering stage. In constraint repair, the the cleaning computations are conducted at repairing stage; the query answering needs no special treatment — any DBMS can be used for its query evaluation. In reality, users are more tolerant with repairing than query answering in terms of time: they usually expect prompt answers to their queries; while they can wait for hours or even days for repairing the dirty data through a batch processing operation. Even when eager approaches (database patching strategy) are used in consistent query answering, performance issue still exists: the evaluation of queries can not take advantages of the well developed database index and optimization techniques because the compact representation of repairs is not stored as normal database tables. Moreover, when the data set is not frequently changed or read only, a physical repair ispreferredd because the same copy of repaired data could be used repeatedly to answer querieswithoutt new effort unless the data is updated. In data mining or data warehousing projects where data quality is a severe problem, complex computations need to be conducted on large set of data. As explained earlier, consistent query answering can hardly support complex queries and large set of data as the same time. Besides the performance concern, in many applications such as data exchange, the users need a physically repaired database.

On the other hand, although the solutions for statistical data editing and imputation can be used to obtain physicrepairsirs of inconsistent data, those solutions are tailored for census/survey data where inconsistencies mostly occur inside a record (tuple) and the major concern for choosing corrections (repair) is not to destroy the statistics. Little work has been done to adapt those solutions to constraint repair.

In constraint repair, functional/inclusion dependencies [BFFR05], denial con-

straints [LB07b] and first order logic [FPL$^+$01] have been studied for characterizing the data. Their focus is the developing of accurate and efficient repairing algorithms. No work has been done to tailor (extend or restrict) traditional constraints in data cleaning context. In the next two chapters of the thesis, a novel extension of functional dependencies is proposed for repair-oriented data cleaning. Efficient algorithms for detecting and repairing inconsistencies in data are presented.

Chapter 3

Modeling the Consistency of Data

One of the most important questions in connection with data cleaning is how to model the consistency of the data, i.e. how to specify and determine that the data is clean? This calls for appropriate application-specific integrity constraints [RD00] to model the fundamental semantics of the data.

As summarized in the last chapter, recent work on data cleaning specifies the consistency of data in terms of constraints, and detects inconsistencies in the data as violations of the constraints. However, previous work on constraint repair is mostly based on traditional dependencies (e.g. functional and full dependencies, etc), which were developed mainly for schema design, but are often insufficient to capture the semantics of the data, as illustrated by the example below.

Example 3.1: A company maintains a relation of customer records:

customer (NAME, CNT, CITY, STR, ZIP, CC, AC, PN).

Each customer tuple contains the NAME, address (country CNT, city CITY, street STR, postal code ZIP) and phone information (country code CC, area code AC, phone number PN) of a customer.

Traditional functional dependencies (FDs) on a customer relation may include:

f_1: [CC, AC, PN] $\rightarrow$ [STR, ZIP, CNT]
f_2: [CNT, ZIP] $\rightarrow$ [CITY]

	NAME	CNT	CITY	STR	ZIP	CC	AC	PN
t_1:	Mike	CA	NYC	Tree Ave.	10012	1	607	1111111
t_2:	Rick	CA	NYC	Tree Ave.	10012	1	607	1111111
t_3:	Joe	US	NYC	Elm Str.	01202	1	212	2222222
t_4:	Jim	US	NYC	Elm Str.	02404	1	212	2222222
t_5:	Ben	US	PHI	Oak Ave.	19014	1	215	3333333
t_6:	Ian	UK	EDI	High St.	EH4 1DT	44	131	4444444

Figure 3.1: An instance of the customer relation

Recall the semantics of an FD: f_1 requires that customer records with the same country code, area code and phone number also have the same street, postal code and country. Similarly, f_2 requires that two customer records with the same country and zip code also have the same city name. Traditional FDs are to hold on all the tuples in the relation (indeed they do on Fig. 3.1).

In contrast, the following constraint is supposed to hold only when the country is UK. That is, for customers in the UK, ZIP determines STR:

ϕ_3: [CNT = UK, ZIP] $\rightarrow$ [STR]

In other words, ϕ_3 is an FD that is to hold on the subset of tuples that satisfies the pattern "CNT = UK", rather than on the entire customer relation. It is generally *not* considered an FD in the standard definition since ϕ_3 includes a *pattern* with *data values* in its specification.

One may think more accurate than [CC, AC, PN] $\rightarrow$ [CNT] in f_1, another traditional functional dependency could be defined as [CC] $\rightarrow$ [CNT]. Unfortunately, this FD doesn't hold on customer relation due to a few exceptions: customers with the same country code of 1 may come from either US or Canada, etc. In real world data, such exceptions often occur and prevent modelling the data using FDs. While these constraints can not be modeled by FD, they may be enforced by:

ϕ_{1a}: [CC = 44] $\rightarrow$ [CNT = UK]

Similar to ϕ_3, many constraints hold on a subset of the tuples instead of all the tuples in a relation. Another example on the customer relation is [CC, AC] $\rightarrow$ [CITY], which does

not hold in US (e.g., for area code 610, the city could be Allentown, Bethlehem, etc.), but holds in UK, China and most other countries:

ϕ_{4a}: [CC = 44, AC] → [CITY]

In US, although it doesn't hold in general, it still holds for some area codes:

ϕ_{4b}: [CC = 1, AC = 212] → [CITY = NYC]
ϕ_{4c}: [CC = 1, AC = 215] → [CITY = PHI]

The following constraints are again not considered FDs:

ϕ_{1b}: [CC = 1, AC = 607, PN] → [STR, ZIP, CNT = US]
ϕ_{2a}: [CNT = US, ZIP = 10012] → [CITY = NYC]
ϕ_{2b}: [CNT = US, ZIP = 19014] → [CITY = PHI]

The first constraint ϕ_{1b} assures that only for country code 1 and area code 607, if two tuples have the same PN, then they must have the same STR and ZIP values and furthermore, the country *must* be US. Similarly, ϕ_{2a} specifies that for all tuples in the us and with zip code 10012, their city must be NYC (irrespective of the values of the other attributes); and ϕ_{2b} assures that if the zip code is 19014 then the city must be PHI.

Observe that ϕ_{1b} *refine* the standard FD f_1 given above, while ϕ_{2a} and ϕ_{2b} refines the FD f_2. This refinement essentially enforces a binding of semantically related data values. Note that while tuples t_1 and t_2 in Fig. 3.1 do not violate f_1, they violate its refined version ϕ_1, since the country cannot be CA if the country code and area code are 1 and 607, respectively. □

In this example, the constraints $\phi_{1a,b}, \phi_{2a,b}, \phi_3, \phi_{4a,b,c}$ capture a fundamental part of the semantics of the data. However, they cannot be expressed as standard FDs and are not considered in previous work on data cleaning. Constraints that hold conditionally may arise in a number of domains. For example, an employee's pay grade may determine her title in some parts of an organization but not in others; an individual's address may determine his tax rate in some countries while in others it may depend on his salary, etc. Further, dependencies that apply conditionally appear to be particularly needed when integrating data, since dependencies that hold only in a subset of sources will hold only conditionally in the integrated data. These call for the study of conditional dependencies, which aim to

capture data inconsistencies at the intentional level (as done in prior work on data cleaning) and extensional level in a *uniform framework*.

In response to the practical need for such constraints, a novel extension of traditional FDs is introduced in next section, referred to as *conditional functional dependencies* (CFDs), that are capable of capturing the notion of "correct data" in these situations. A CFD extends an FD by incorporating a pattern tableau that enforce binding of semantically related values. Unlike its traditional counterpart, the CFD is required to hold only on tuples that satisfy a pattern in the pattern tableau, rather than on the entire relation. For examples, all the constraints we have encountered so far can be expressed as CFDs.

3.1 Conditional Functional Dependencies

In this section we define conditional functional dependencies (CFDs). Consider a relation schema R defined over a fixed set of attributes, denoted by $\mathtt{attr}(R)$.

Syntax. A CFD φ on R is a pair $(R : X \rightarrow Y,\ T_p)$, where (1) X, Y are sets of attributes from $\mathtt{attr}(R)$, (2) $R : X \rightarrow Y$ is a standard FD, referred to as the FD *embedded in* φ; and (3) T_p is a tableau with all attributes in X and Y, referred to as the *pattern tableau* of φ, where for each A in X or Y and each tuple $t \in T_p$, $t[A]$ is either a constant 'a' in the domain $\mathsf{dom}(A)$ of A, or an unnamed variable '_'.

If A occurs in both X and Y, we use $t[A_L]$ and $t[A_R]$ to indicate the occurrence of A in X and Y, respectively, and separate the X and Y attributes in a pattern tuple with '$\|$'. We write φ as $(X \rightarrow Y,\ T_p)$ when R is clear from the context.

Example 3.2: The constraints $\phi_{1a,b}, \phi_{2a,b}, \phi_3$, $\phi_{4a,b,c}$ on the customer table given in Example 3.1 can be expressed as CFDs φ_1 (for ϕ_{1a} and ϕ_{1b}, from the second line one per line, respectively), φ_2 (for ϕ_{2a} and ϕ_{2b}), φ_3 (for ϕ_3), and φ_4 (for ϕ_{4a}, ϕ_{4b}, and ϕ_{4c}, one per line), as shown in Fig. 3.2. In fact all the constraints we have encountered so far can be expressed as CFDs. Indeed, the traditional functional dependencies f_1 and f_2 are expressed by the first pattern tuple of CFDs φ_1 and φ_2 given in Fig. 3.2, respectively. □

If we represent both data and constraints in a uniform tableau format, then at one end of the spectrum are relational tables which consist of data values without logic variables, and at the other end are traditional constraints which are defined in terms of logic variables

$T_1 =$

CC	AC	PN	STR	ZIP	CNT
_	_	_	_	_	_
44	_	_	_	_	UK
1	607	_	_	_	US

(a) $\varphi_1 = ([\mathsf{CC}, \mathsf{AC}, \mathsf{PN}] \rightarrow [\mathsf{STR}, \mathsf{ZIP}, \mathsf{CNT}], T_1)$

$T_2 =$

CNT	ZIP	CITY
_	_	_
US	10012	NYC
US	19014	PHI

(b) $\varphi_2 = ([\mathsf{CNT}, \mathsf{ZIP}] \rightarrow [\mathsf{CITY}], T_2)$

$T_4 =$

CC	AC	CITY
44	_	_
1	212	NYC
1	215	PHI

(c) $\varphi_4 = ([\mathsf{CC}, \mathsf{AC}] \rightarrow [\mathsf{CITY}], T_4)$

$T_3 =$

CNT	ZIP	STR
UK	_	_

(d) $\varphi_3 = ([\mathsf{CNT}, \mathsf{ZIP}] \rightarrow [\mathsf{STR}], T_3)$

Figure 3.2: Example CFDs

but without data values, while CFDs are in the between.

Semantics. Intuitively, the pattern tableau T_p of φ refines the standard FD embedded in φ by enforcing the binding of semantically related data values. To define the semantics of φ, we first introduce a notation. For a pattern tuple t_p in T_p, we define an *instantiation* ρ to be a mapping from t_p to a *data tuple* with no variables, such that for each attribute A in $X \cup Y$, if $t_p[A]$ is '_', ρ maps it to a constant in $\mathsf{dom}(A)$, and if $t_p[A]$ is a constant 'a', ρ maps it to the *same* value 'a'. For example, for $t_p[A,B] = (a, \_)$, one can define an instantiation ρ such that $\rho(t_p[A,B]) = (a,b)$, which maps $t_p[A]$ to itself and $t_p[B]$ to a value b in $\mathsf{dom}(B)$. Obviously, for an attribute A occurring in both X and Y, we require that $\rho(t_p[A_L]) = \rho(t_p[A_R])$.

A data tuple t is said to *match* a pattern tuple t_p, denoted by $t \asymp t_p$, if there is an instantiation ρ such that $\rho(t_p) = t$. For example, $t[A,B] = (a,b) \asymp t_p[A,B] = (a, \_)$.

A relation I of R *satisfies* the CFD φ, denoted by $I \models \varphi$, if for *each pair* of tuples t_1, t_2 in the relation I, and for *each* tuple t_p in the pattern tableau T_p of φ, if $t_1[X] = t_2[X] \asymp t_p[X]$, then $t_1[Y] = t_2[Y] \asymp t_p[Y]$. That is, if $t_1[X]$ and $t_2[X]$ are equal and in addition, they both

match the pattern $t_p[X]$, then $t_1[Y]$ and $t_2[Y]$ must also be equal to each other and both match the pattern $t_p[Y]$. Moreover, if Σ is a set of CFDs, we write $I \models \Sigma$ if $I \models \varphi$ for *each* CFD $\varphi \in \Sigma$. If a relation $I \models \Sigma$, then we say that I is *clean* with respect to Σ.

Example 3.3: The customer relation in Fig. 3.1 satisfies φ_2, φ_3 and φ_4 of Fig. 3.2. However, it does not satisfy φ_1. Indeed, tuple t_1 *violates* the pattern tuple $t_p = (\texttt{01, 607, \_} \,\|\, \texttt{\_, \_, US})$ in tableau T_1 of φ_1: $t_1[\mathsf{CC}, \mathsf{AC}, \mathsf{PN}] = (\texttt{01, 607, 1111111}) \asymp (\texttt{01, 607, \_})$, but $t_1[\mathsf{STR}, \mathsf{ZIP}, \mathsf{CNT}] = (\texttt{Tree Ave., 07974, CA}) \not\asymp (\texttt{\_, \_, US})$ since $t_1[\mathsf{CNT}]$ is `CA` instead of `US`; similarly for t_2. □

This example tells us that while violation of a standard FD requires *two* tuples, a *single* tuple may violate a CFD.

Two special cases of CFDs are worth mentioning. First, a standard FD $X \to Y$ can be expressed as a CFD $(X \to Y,\ T_p)$ in which T_p contains a single tuple consisting of '_' only. For example, if we let T_2 of φ_2 in Fig. 3.2 contain only $(\_, \_ \,\|\, \_)$, then it is the CFD representation of the FD f_2 given in Example 3.1. Second, an instance-level FD $X \to Y$ studied in [LSPR96] is a special CFD $(X \to Y,\ T_p)$, where T_p contains a single tuple consisting of only data values.

Observe that pattern tableaux in CFDs are quite different from Codd tables, variable tables and conditional tables, which have been traditionally used in the context of incomplete information [IJ84, Gra91]. The key difference is that each of these tables represents possibly infinitely many relation instances, one instance for each instantiation of variables. No instance represented by these table formalisms can include two tuples that result from different instantiations of a table tuple. In contrast, a pattern tableau is used to constrain–as part of a CFD–a *single* relation instance, which can contain any number of tuples that are all instantiations of the same pattern tuple via different valuations of the unnamed variables '_'.

Normal form. From the semantics of CFDs we immediately obtain a *normal form* of CFDs: Given a set Σ of CFDs, we may assume that each CFD $\phi \in \Sigma$ is of the form $\phi = (R : X \to A, t_p)$, where $A \in \mathsf{attr}(R)$ and t_p is a single pattern tuple. For ease of exposition we assume that CFDs are given in the normal form.

Satisfiability. To clean data based on CFDs we need to make sure that the CFDs are satisfiable, or make sense. The *satisfiability problem* is to determine, given a set Σ of CFDs,

whether or not there exists a (non-empty) database D such that $D \models \Sigma$. While this problem is trivial for traditional FDs, i.e. any set of FDs is satisfiable, this is no longer true for CFDs. Indeed, it has been shown that this problem is intractable in general [BFG$^+$07, FGJK08]. However, when the database schema is fixed, satisfiability of CFDs can be decided in PTIME [BFG$^+$07, FGJK08]. In the sequel we consider satisfiable CFDs only.

3.2 Detecting CFD Violations

A first step for data cleaning is the efficient detection of constraint violations in the data. In this section we develop techniques to detect violations of CFDs. Given an instance I of a relation schema R and a set Σ of CFDs on R, it is to find all the *violating tuples* in I, i.e. the tuples that (perhaps together with other tuples in I) violate some CFD in Σ. We first provide an SQL technique for finding violations of a single CFD, and then present an incremental technique for validating CFDs. It is desirable to use *just* SQL to find violations: this makes detection feasible in any standard relational DBMS without requiring any additional functionality on its behalf.

3.2.1 Checking a CFD with SQL

Consider a CFD $\varphi = (X \rightarrow A,\ T_p)$. A naïve approach to find the tuples violating φ is demonstrated by the following example:

Example 3.4: Given φ_4 = ([CC,AC] $\rightarrow$ [CITY], T_4) shown in 3.2. Naïvely, we can issue three SQL queries, one for each pattern tuple $t_p \in T_4$, to identity inconsistent tuples in a customer instance:

$Q^1_{\varphi_4}$ **select distinct** AC **from** customer t
where t[CC] =‘44’
group by AC **having count** (**distinct** CITY)> 1

$Q^2_{\varphi_4}$ **select** * **from** customer t
where t[CC] =‘1’ **and** t[AC] =‘212’ **and** t[CITY] <>‘NYC’

$Q^3_{\varphi_4}$ **select** * **from** customer t
where t[CC] =‘1’ **and** t[AC] =‘215’ **and** t[CITY] <>‘PHI’

Although each query in the above example is very efficient providing proper indice have been created for the customer relation, the number of the queries — which equals to the number of tuples in the pattern tableau — could be huge. Since CFD allows the binding of values, the cardinality of a CFD could easily grow very large in practice. For example, to achieve precise checking of the consistency between postal codes and addresses, one may create a large pattern tableau containing all the mappings of postal codes and addresses in a country or even for the world. Such a pattern tableau could even be larger than the database instance.

Is there a way to detect CFD violations without using potentially large number of SQL queries? Let's look at a different query to find the tuples violating φ_3 by directly following the CFD definition:

Q_{φ_4} **select** t1.* **from** customer t_1, customer t_2, T_4 t_p
where $t_1[\mathsf{CC}] = t_2[\mathsf{CC}] \asymp t_p[\mathsf{CC}]$ **and** $t_1[\mathsf{AC}] = t_2[\mathsf{AC}] \asymp t_p[\mathsf{AC}]$
and not ($t_1[\mathsf{CITY}] = t_2[\mathsf{CITY}] \asymp t_p[\mathsf{CITY}]$)

where $t_1[\mathsf{CC}] = t_2[\mathsf{CC}] \asymp t_p[\mathsf{CC}]$ is a short-hand for the SQL expression ($t_1[\mathsf{CC}]$ = $t_2[\mathsf{CC}]$ **and** ($t_2[\mathsf{CC}]$ = $t_p[\mathsf{CC}]$ **or** $t_p[\mathsf{CC}]$ = '_')), and similarly for $t_1[\mathsf{AC}] = t_2[\mathsf{AC}] \asymp t_p[\mathsf{AC}]$ and $t_1[\mathsf{CITY}] = t_2[\mathsf{CITY}] \asymp t_p[\mathsf{CITY}]$.

Obviously, this single query is enough to detect all the violations in a customer instance against CFD φ_4 irrespective to the size of the CFD, because the pattern tableau T_4 is treated as an ordinary data table. These pattern tables are dynamically created when a CFD with a new embedded FD is specified. Since the number of pattern tuples could be larger than the cardinality of the relation instance as explained earlier, the size of the SQL query in the Naïve approach may exceed the relation instance. So the communication time for sending these queries could grow as high as to transfer the relation instance, not to mention that it is not feasible to keep the queries in memory. In other words, the Naïve approach encodes the potential huge domain knowledge in the queries. Now the domain knowledge is stored in the database and only a small SQL query is needed for checking CFD violations. As a result, the communication time is reduced dramatically by the compactness of the query. However, this compact query is very costly. The self-join of customer relation is an expensive operation which causes the poor performance.

Thus, it is natural to ask if there is an approach to detect CFD violations which combines the advantages of both methods above, i.e., an approach to compose a set of concise queries, irrespective to the size of the CFD, that can efficiently find the inconsistent tuples in an instance against a CFD without expensive joins?

By analyzing the above queries, we find that to achieve this goal we should: (1) separate the detection of single-tuple violations (i.e. the tuples violating the bound values in the pattern tableau of a CFD) and multi-tuple violations (i.e. the sets of tuples in which each set mutually violate at least one pattern tuple with '_' at RHS); (2) favor the "group by" operations and avoid using the self-join. □

Follows the above guidance, we found a way to compose efficient queries to detect CFD violations. Given a CFD $\varphi = (X \rightarrow A,\ T_p)$, the following two SQL queries suffice to find the tuples violating φ:

Q^C_φ **select** * **from** $R\ t,\ T_p\ t_p$
where $t[X] \asymp t_p[X]$ **and** $t[A] \not\asymp t_p[A]$

Q^V_φ **select distinct** X **from** $R\ t,\ T_p\ t_p$
where $t[X] \asymp t_p[X]$ **and** $t_p[A] =$ '_'
group by X **having count** (**distinct** A)> 1

where for an attribute $B \in (X \cup A)$, $t[B] \asymp t_p[B]$ is a short-hand for the SQL expression ($t[B]$ = $t_p[B]$ **or** $t_p[B]$ = '_'), while $t[B] \not\asymp t_p[B]$ is a short-hand for ($t[B] \neq t_p[B]$ **and** $t_p[B] \neq$ '_').

Intuitively, detection is a two-step process, each conducted by a query. Initially, query Q^C_φ detects *single-tuple* violations, i.e. the tuples t in I that match some pattern tuple $t_p \in T_p$ on the X attributes, but t does not match t_p in A since the *constant* value $t_p[A]$ is different from $t[A]$. That is, Q^C_φ finds violating tuples based on differences in the constants in the tuples and T_p patterns.

On the other hand, query Q^V_φ finds *multi-tuple* violations, i.e. tuples t in I for which there exists a tuple t' in I such that $t[X] = t'[X]$ and moreover, both t and t' match a pattern t_p on the X attributes, value $t_p[A]$ is a variable, but $t[A] \neq t'[A]$. Query Q^V_φ uses the **group by** clause to group tuples with the same value on X and it counts the number of distinct instantiations in $t_p[A]$. If there is more than one instantiation, then there is a violation. Note that Q^V_φ returns only the X attributes of violating tuples. This has the advantage that the output

$Q^C_{\varphi_1}$ **select** * **from** customer t, T_1 t_p
where $t[\mathsf{CC}] \asymp t_p[\mathsf{CC}]$ **and** $t[\mathsf{AC}] \asymp t_p[\mathsf{AC}]$ **and** $t[\mathsf{PN}] \asymp t_p[\mathsf{PN}]$ **and**
($t[\mathsf{STR}] \not\asymp t_p[\mathsf{STR}]$ **or** $t[\mathsf{ZIP}] \not\asymp t_p[\mathsf{ZIP}]$ **or** $t[\mathsf{CNT}] \not\asymp t_p[\mathsf{CNT}]$)

$Q^V_{\varphi_1}$ **select distinct** CC, AC, PN **from** customer t, T_1 t_p
where $t[\mathsf{CC}] \asymp t_p[\mathsf{CC}]$ **and** $t[\mathsf{AC}] \asymp t_p[\mathsf{AC}]$ **and** $t[\mathsf{PN}] \asymp t_p[\mathsf{PN}]$ **and**
($t_p[\mathsf{STR}] =$ '_' **or** $t_p[\mathsf{ZIP}] =$ '_' **or** $t_p[\mathsf{CNT}] =$ '_')
group by CC, AC, PN **having count** (**distinct** STR, ZIP, CNT)> 1

Figure 3.3: SQL queries for checking CFD φ_1

is more concise than when we would return the complete tuples. Moreover, the complete tuples can be easily obtained using an additional SQL query.

This solution can be trivially extended to multiple attributes, as illustrated in the following example:

Example 3.5: Recall CFD φ_1 given in Fig. 3.2. Over a customer instance I, the SQL queries $Q^C_{\varphi_1}$ and $Q^V_{\varphi_1}$ shown in Fig. 3.3 determine whether or not I satisfies φ_1. Executing these queries over the instance of Fig. 3.1, it returns tuples t_1, t_2 (due to $Q^C_{\varphi_1}$), and t_3 and t_4 (due to $Q^V_{\varphi_1}$). □

A salient feature of our SQL translation is that tableau T_p is treated an ordinary data table. Therefore, each query is bounded by the size of the embedded FD $X \rightarrow A$ in the CFD, and is *independent* of the size (and contents) of the (possibly large) tableau T_p.

3.2.2 Incremental CFD Detection

Consider an instance I of a relation schema R and a CFD $\varphi = (X \rightarrow A,\ T_p)$. Given the methodology presented thus far, we can check for violations of φ by issuing the pair of queries Q^C_φ and Q^V_φ over I. An interesting questions is then what happens if the instance I changes? As tuples are inserted or deleted from I, resulting a new instance I^{new}, a naive solution would be a batch approach that re-issues queries Q^C_φ and Q^V_φ over I^{new}, starting from scratch in response to updates, something that requires two passes of the underlying instance each time the queries are re-issued.

Intuitively, however, one expects that a tuple insertion leaves a large portion of instance I unaffected when CFD violations are concerned. An inserted tuple t might introduce *new* violations, but only with tuples that are already in the instance and match t in the X attributes. Therefore, it makes sense to *only* access these tuples and *only* detect the possible newly introduced violations due to the inserted tuple. Thus, *incremental* detection can potentially save a large number of disk accesses, since instead of performing two passes of the underlying data on each tuple insertion (naive method), we only need to access the tuples that match the inserted tuple t in the X attributes. Similarly in the case of deletion, by deleting a tuple t we might inadvertibly *repair* some of the violations in I that the deleted tuple was causing (again with tuples matching t in the X attributes). Therefore, it makes sense to *only* detect which of the existing violations concerning the deleted tuple are affected. The following example better illustrates the above.

Example 3.6: Recall from Example 3.5 that tuples t_1 to t_4 in Fig. 3.1 violate CFD φ_1. Now, consider inserting the tuple t_7 : (`Bill, US, PHI, Main Rd., 19014, 01, 215, 3333333`) in the relation of the figure. It is easy to check that tuples t_5 and t_7 violate φ_1 (due to $Q^V_{\varphi_1}$). Still, the newly inserted tuple does not affect the violations detected between the first four tuples. Note that an incremental detection would require that we only access tuple t_5, instead of the whole relation.

Now, consider again the instance in Fig. 3.1 and assume that we delete tuple t_4 from it. Then, it is easy to check that tuple t_3 no longer violates φ_1 since the deletion of t_4 inadvertibly repaired the violation caused by tuples t_3 and t_4. At the same time, note that such a deletion only requires accessing tuple t_3 and does not affect the violation caused by tuples t_1 and t_2. □

We next present a method to *incrementally* detect CFD violations, given a set of insertions and deletions to an instance I. Although the incremental method has the same worst-case performance as the naive method (two passes of the underlying instance), its expected performance is that only a small number of tuples are accessed, which will be verified in the next section by our experiments.

	NAME	CNT	CITY	STR	ZIP	CC	AC	PN	$\beta^C_{\varphi_1}$	$\beta^V_{\varphi_1}$
t_1:	Mike	CA	NYC	Tree Ave.	10012	1	607	1111111	1	0
t_2:	Rick	CA	NYC	Tree Ave.	10012	1	607	1111111	1	0
t_3:	Joe	US	NYC	Elm Str.	01202	1	212	2222222	0	1
t_4:	Jim	US	NYC	Elm Str.	02404	1	212	2222222	0	1
t_5:	Ben	US	PHI	Oak Ave.	19014	1	215	3333333	0	0
t_6:	Ian	UK	EDI	High St.	EH4 1DT	44	131	4444444	0	0

Figure 3.4: The customer relation instance with logging information

3.2.2.1 Logging of violations

The incremental detection requires us to extend the schema R of an instance relation I to record which tuples violate which CFDs in a given set Σ. In more detail, for each CFD $\varphi \in \Sigma$ we add two Boolean attributes β^C_φ and β^V_φ to the schema of R. We use R^{log} to denote the new schema. For each tuple $t \in I$, we create a tuple t' in R^{log} such that $t'[\mathsf{attr}(R)] = t[\mathsf{attr}(R)]$. Furthermore, in attribute $t'[\beta^C_\varphi]$ (resp. $t'[\beta^V_\varphi]$) we record whether or not the corresponding tuple t violates CFD φ due to Q^C_φ (resp. Q^V_φ). Note that our logging mechanism imposes minimum overhead, in terms of space, since for each tuple and each CFD only two additional bits are required.

We assume that, initially, we execute queries Q^C_φ and Q^V_φ and we use the result of the two queries to initialize the values of attributes β^C_φ and β^V_φ, through a simple SQL update statement of the following form for β^C_φ (similarly for β^V_φ):

U^C_φ **update** R^{log} t' **set** $t'[\beta^C_\varphi] = 1$
where $t'[\mathsf{attr}(R)]$ **in** (Q^C_φ)

One needs only to select all those tuples with both β^C_φ and β^V_φ equal to false, for each $\varphi \in \Sigma$, and then project on $\mathsf{attr}(R)$, in order to retrieve from R^{log} the tuples that do not violate any of the CFDs. Figure 3.4 shows the instance of Fig. 3.1 after its schema has been extended appropriately to log violations for CFD φ_1.

3.2.2.2 Handling tuple deletions

We use SQL statements to detect violations, in an incremental fashion. Consider a CFD $\varphi = (X \rightarrow A,\ T_p)$ and an instance I^{log} whose schema R^{log} includes attributes β_φ^C and β_φ^V. In response to deletion of tuple t from I^{log}, the incremental detection of violations has two simple steps.

Step 1: **delete from** $R^{log}\ t'$ **where** $t' = t$

Step 2: **update** $R^{log}\ t'$ **set** $t'[\beta_\varphi^V] = 0$
where $t'[\beta_\varphi^V] = 1$ **and** $t'[X] = t[X]$ **and**
$1 =$ (**select count** (**distinct** A) **from** $R^{log}\ t''$
where $t''[X] = t[X]$)

In more detail, the SQL query in the first step simply deletes from R^{log} the tuple corresponding to t. The second step checks for tuples that (a) violate φ ($t'[\beta_\varphi^V] = 1$), (b) have the same values on the X attributes with t, and (c) all these identified tuples have the same A attribute value. It is easy to see that if a set of tuples satisfies the above three conditions, then each of the tuples in the set violated φ only due to t. Since we delete t, each of the tuples now satisfies φ. Therefore, we set $t'[\beta_\varphi^V]$ to false. Note that a tuple deletion only affects violations that are caused by the presence of '_' in the tableau, hence we focus only on the β_φ^V attribute. Also note that the above procedure need not access the pattern tableau T_p of φ, resulting in additional savings in terms of execution time.

Example 3.7: Consider the instance in Fig. 3.4 and assume that we delete tuple t_4. Then the second step of our incremental detection will select tuple t_3 and set $t_3[\beta_{\varphi_1}^V]$ to false since there is no other tuple in the instance that has the same values on the CC, AC and PN attributes as t_3 but differs from t_3 in STR, CT or ZIP. Hence tuple t_3 no longer violates φ_1. Note that our incremental detection, using appropriate indexes, only accesses tuple t_3. In contrast the non-incremental detection requires to access the whole relation twice. □

An interesting question is what happens when we want to do *batch* deletion, i.e., delete a set of tuples. Obviously, we could execute the above two steps once for each tuple in the set. We can actually do better than that since it suffices to execute the above steps once for each *distinct* value of X attributes that is deleted. So, if for example we delete both tuples t_3 and t_4 from the instance in Fig. 3.4, we only need to execute the two steps once since

the two tuples have the same value on the X attributes. This simple observation provides additional savings.

3.2.2.3 Handling tuple insertions

Assume that we want to insert a tuple t into I^{log}. Then, the incremental detection of violations has the following three steps.

Step 1: **insert into** R^{log} **values** t

Step 2: **update** R^{log} t' **set** $t'[\beta_\varphi^C] = 1$
where $t' = t$ **and**
exists (**select** * **from** T_p
where $t_p[X] \asymp t'[X]$ **and** $t_p[A] \not\asymp t'[A]$)

Step 3: **update** R^{log} t' **set** $t[\beta_\varphi^V] = 1, t'[\beta_\varphi^V] = 1$
where $t'[X] = t[X]$ **and** $t'[A] \neq t[A]$ **and**
exists (**select** * **from** T_p t_p
where $t_p[X] \asymp t[X]$ **and** $t_p[A] =$ '_')

The first step simply inserts the tuple t into relation R^{log}, where we assume that both the β_φ^C and β_φ^V attributes are set to false, for each newly inserted tuple. Similar to Q_φ^C, the second step checks for violations in the constants between the recently inserted tuple and the pattern tableau T_p. If such violations exist, it sets the value of β_φ^C in the inserted tuple to true. Similar to Q_φ^V, the final step checks for tuples that (a) have the same values on the X attributes with t, (b) differ from t on the A attribute, and (c) the pattern tuple matching t has value '_' for A attribute. It is not hard to see that if the above conditions are satisfied, each identified tuple and t, when put together, violate φ. Therefore, we set the value of the β_φ^V attribute of each such tuple to true. We slightly abuse notation in this last step to also update, with the same statement, the value of the β_φ^V attribute of t to true.

We now consider batch insertions involving a set of tuples, say ΔI^{log}. Obviously, one might consider executing the above steps once for each tuple in ΔI^{log}. An alternative strategy is to treat ΔI^{log} as an independent instance whose tuples we need to merge with the ones in I^{log}. We distinguish five different steps here:

Step 1: **update** $\Delta R^{log}\ t'$ **set** $t'[\beta_\varphi^C] = 1$
where $t'[\mathsf{attr}(R)]$ **in** (Q_φ^C)

Step 2: **update** $R^{log}\ t'$ **set** $t'[\beta_\varphi^V] = 1$
where $t'[\beta_\varphi^C] = 0$ **and** $t'[\beta_\varphi^V] = 0$ **and**
exists (**select** * **from** $T_p\ t_p$
where $t_p[X] \asymp t[X]$ **and** $t_p[A] =$ '_') **and**
exists (**select** * **from** $\Delta R^{log}\ t''$
where $t''[X] = t'[X]$ **and** $t''[A] \neq t'[A]$) **and**

Step 3: **update** $\Delta R^{log}\ t'$ **set** $t'[\beta_\varphi^V] = 1$
where **exists** (**select** * **from** $R^{log}\ t''$
where $t''[X] = t'[X]$ **and** $t''[\beta_\varphi^V] = 1$)

Step 4: **update** $\Delta R^{log}\ t'$ **set** $t'[\beta_\varphi^V] = 1$
where $t'[\beta_\varphi^C] = 0$ **and** $t'[\beta_\varphi^V] = 0$ **and**
$t'[X]$ **in** (**select** X **from** $\Delta R^{log}\ t''$, $T_p\ t_p$
where $t''[\beta_\varphi^C] = 0$ **and** $t''[\beta_\varphi^V] = 0$ **and** $t''[X] \asymp t_p[X]$
$t_p[A] =$ '_'
group by X
having count (**distinct** A)> 1)

Step 5: **insert into** R^{log} **values** (**select** * **from** ΔR^{log})

where ΔR^{log} denotes the schema of ΔI^{log}, which is identical to R^{log}. During the first step, we focus on the newly inserted tuples and we identify which tuples independently violate φ due to Q_φ^C. This is an unavoidable step whose cost cannot be reduced since we have to consider each inserted tuple in isolation. However, by executing Q_φ^C only over ΔR^{log}, we avoid re-detecting such violations over R^{log}.

The second step looks for tuples in R^{log} that were clean before the insertion of tuples in ΔR^{log} but will now violate φ, once the tuples in ΔR^{log} are inserted. The tuples in R^{log} that are affected by the insertion are such that they have the same values on the X attributes with some tuple in ΔR^{log} but their values differ on the A attribute.

	NAME	CNT	CITY	STR	ZIP	CC	AC	PN	$\beta^C_{\varphi_1}$	$\beta^V_{\varphi_1}$
t_7:	Tim	CA	NYC	Main Str.	01202	1	607	5555555	0	0
t_8:	Sam	US	NYC	Elm Str.	01202	1	212	2222222	0	0
t_9:	Al	UK	EDI	King St.	EH4 1DT	44	131	4444444	0	0

Figure 3.5: An instance ΔI^{log} used for batch insertion

The third step attempts to leverage the knowledge of violations in R^{log} in order to detect violations in ΔR^{log}. In more detail, if a tuple t' in ΔR^{log} has the same values on the X attributes with some tuple t'' in R^{log} whose β^V_φ is true, then t' must also have β^V_φ set to true. This is because we already know for the tuples in R^{log} with specific values on the X attributes whether or not more than one values on the A attribute exist.

Finally, there is only one more case to consider, namely, whether there are any *clean* tuples in ΔR^{log} (with both β^C_φ and β^V_φ equal to false) that together with some other clean tuples in ΔR^{log} violate φ. The last step detects such tuples by checking whether any tuples have the same values on the X attributes but different values on the A attribute. For all the detected tuples, the value of β^V_φ is set to true.

In last step, we simply insert the tuples in ΔR^{log} into R^{log}.

Example 3.8: Consider the instance in Fig. 3.5 and assume that we want to insert its tuples to the instance in Fig. 3.4. Then, the first step above will set $t_7[\beta^C_{\varphi_1}]$ to true, since the value of $t_7[\mathsf{CNT}]$ is "CA" instead of "US". The second step will set $t_6[\beta^V_{\varphi_1}]$ to true, since tuples t_6 and t_9 violate φ_1. The third step will set $t_9[\beta^V_{\varphi_1}]$ also to true, while none of the remaining steps will alter any tuples. □

3.3 Experimental Study: Detecting CFD Violations

In this section, we present our findings about the performance of our techniques for (incrementally) detecting CFD violations over a variety of data sizes, and number and complexity of CFDs. We distinguish three sets of experiments. After identifying a number of parameters that influence the detection of violations, in the first set of experiments we vary these parameters, and we investigate the effects of each parameter combination on the execution

time of the SQL detection queries. In the second set of experiments, we focus on the detection of multiple CFDs and we study the benefits of merging multiple CFDs in a single tableau. It is important to note that in the first two sets of experiments we *only* report the time to execute the SQL detection queries and omit the time to report (or *mark*) the violating tuples. This omission does not affect the validity of our results since, for the first two sets of experiments, marking the violating tuples only adds a constant to each reported time of each figure. However, this overhead is important in the third set of experiments where we focus on incremental detection and its benefits with respect to the non-incremental one. There, the reported times are the sum of the time to execute the SQL detection query plus the time to mark the violating tuples.

3.3.1 Experimental Setup

− **Hardware:** For the experiments, we used DB2 on an Apple Xserve with 2.3GHz PowerPC dual CPU and 4GB of RAM.

− **Data:** Our experiments used an extension of the relation in Fig. 3.1. Specifically, the relation models individual's tax-records and includes 8 additional attributes, namely, the state ST where a person resides, her marital status MR, whether she has dependents CH, her salary SA, tax rate TX on her salary, and 3 attributes recording tax exemptions, based on marital status and the existence of dependents.

To populate the relation we collected real-life data: the zip and area codes for major cities and towns for all US states. Further, we collected the tax rates, tax and income brackets, and exemptions for each state. Using these data, we wrote a program that generates synthetic tax records.

We vary two parameters of the data instance in our experiments, denoted by SZ and NOISE. SZ determines the tuple number in the tax-records relation and NOISE the percentage of dirty tuples. We randomly introduce errors in the data. More specifically, as the data is generated, with probability NOISE, an attribute on the RHS of a CFD is changed from a correct to incorrect value (e.g. a tax record for a NYC resident with a Chicago area code). The schema of the generated relation is: tax_records (RID, DIRTY, FNAME, LNAME, AC, PN, CITY, STATE, ZIP, MARITAL, CHILD, SALARY, TAXRATE, SINEXEMPT, MAREXEMPT, CHIEXEMPT). Each tax_records tuple contains the record id, the dirty

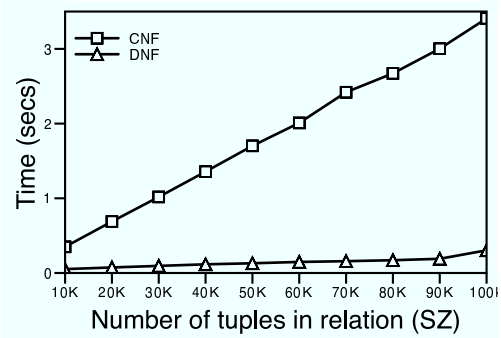
tag, the tax payer's first name, last name, area code, phone number, city name, state name, zip code, marital status, number of children, salary, tax rate, single person exemption, married exemption, and children exemption. The dirty tag attribute is to help verify whether all of the tuples with noises are detected as inconsistent tuples.

– **CFDs:** We used CFDs to model real-world semantics such as (a) zip codes determine states, (b) zip codes and cities determine states. (c) states and salary brackets determine tax rates (a tax rate depends on both the state and employee salary), etc. We varied our CFDs using the following parameters: NUMCFDs determined the number of CFDs considered in an experimental setup, NUMATTRs the (max) attribute number in the CFDs, TABSZ the (max) tuple number in the CFDs, and NUMCONSTs the percentage of tuples with constants vs. tuples with variables in each CFD.

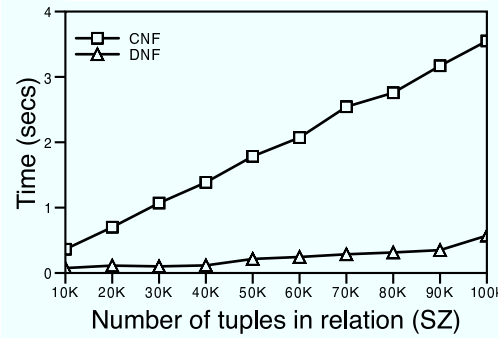
3.3.2 Detecting CFD Violations

There are two alternative evaluation strategies for the SQL detection queries of Section 3.2. Key distinction between these two strategies is how we evaluate the **where** clause in each detection query. Specifically, note that the **where** clause of our SQL detection queries is in conjunctive normal form (CNF). It is known that database systems do not efficiently execute queries in CNF since the presence of the OR operator leads the optimizer to select inefficient plans that do not leverage the available indexes. A solution to this problem is to convert conditions in the **where** clause into disjunctive normal form (DNF). This conversion might cause an exponential blow-up in the number of conjuncts, but in this case, the blow-up is *w.r.t.* the number of attributes in the CFD, which is usually very small.

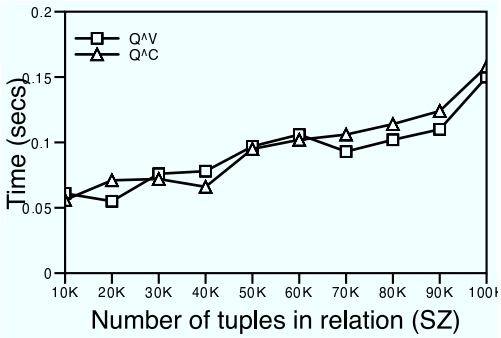
– CNF **vs.** DNF**:** In this experiment, we considered both evaluation strategies, under various settings, to determine the most efficient one. In more detail, we considered relations with SZ from 10K to 100K tuples, in 10K increments, and 5% NOISE. We considered two *representative* CFDs, each with NUMATTRs 3, where the first CFD had NUMCONSTs 100% (tuples with only constant) while the second had NUMCONSTs 50% (half the tuples had variables). In terms of CFD size, we set TABSZ to 1K (note that *each tuple* in the CFDs is a constraint itself). Figures 3.6(a) and 3.6(b) show the evaluation times for both evaluation strategies, for each of the two CFDs. As both graphs show, irrespective of data size and the presence of constants or variables, the DNF strategy clearly out-performs the CNF one.



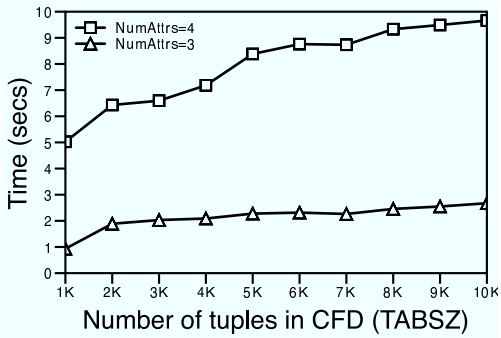
(a) CNF vs DNF (NUMCONSTs = 100%)



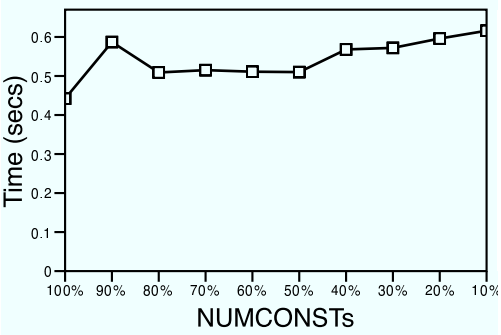
(b) CNF vs DNF (NUMCONSTs = 50%)



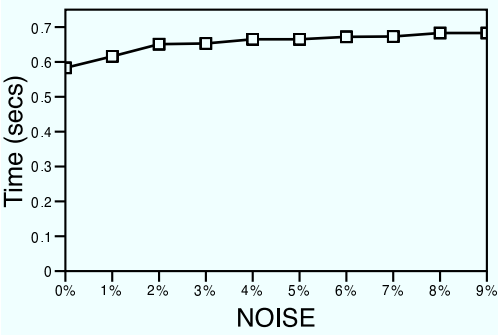
(c) Q^C_φ vs. Q^V_φ



(d) Scalability in TABSZ



(e) Scalability in NUMCONSTs



(f) Scalability in NOISE

Figure 3.6: Experimental results

Furthermore, the figures illustrate the scalability of our detection queries SZ.

– Q^C_φ **vs.** Q^V_φ**:** In this experiment, we investigated how the detection time is split between the Q^C_φ and Q^V_φ queries. We considered relations with SZ from 10K to 100K tuples, in 10K

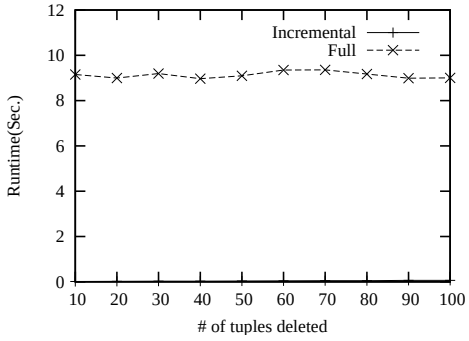
increments, and 5% NOISE. For the CFD, we consider one with NUMATTRs equal to 3, TABSZ to 1K and NUMCONSTs 100% (we made similar observations for other values of NUMCONSTs). Figure 3.6(c) shows the evaluation times for each query in isolation and shows that both queries have similar loads and they follow the same execution trend.

– **Scalability in** TABSZ**:** Here, we study the scalability of the detection queries with respect to TABSZ. In more detail, we fixed SZ to 500K with 5% NOISE. We considered two CFDs whose sizes varied from 1K to 10K, in 1K increments. The NUMATTRs was 3 for the first, and 4 for the second CFD considered. For all CFDs, NUMCONSTs was 50%. Figure 3.6(d) shows the detection times for the 2 CFDs. As is obvious from the figure, TABSZ has little impact on the detection times and dominant factors here are (a) the size of the relation, which is much larger than the tableaux, and (b) the number of attributes in the tableau, since these result in more complicated join conditions in the detection queries.

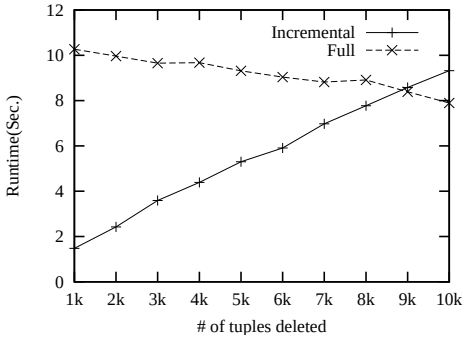
– **Scalability in** NUMCONST**s:** We studied the impact of variables on the detection times. We considered a relation with SZ 100K and NOISE 5% and a CFDs with TABSZ 1K, and NUMATTRs = 3. We varied NUMCONSTs between 100% (all constants) and 10% and we measured the detection times over the relation. Figure 3.6(e) shows that variables do affect detection times and (not shown in the figure) moreover, as we increased both the percentage of variables and the number of attributes with variables, detection times increased noticeably. This is apparent, given that variables restrict the use of indexes while joining the relation with the tableau.

– **Scalability in** NOISE**:** Here, we varied NOISE between 0% and 9% in a relation with SZ 100K, and we measured detection time, for a CFD with TABSZ 30K (we used all possible zip to state pairs, so as not to miss a violation), NUMATTRs 2, and NUMCONSTs 100%. As we can see in Fig. 3.6(f), the level of NOISE has negligible effects on detection times.

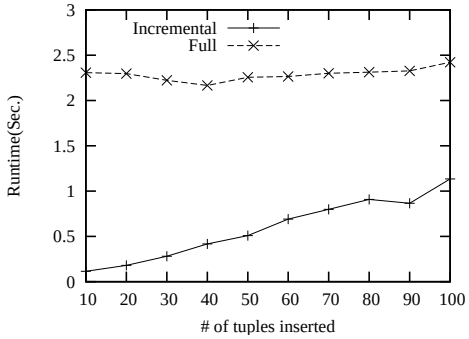
– **On the representation of variables:** One practical consideration, during our experiments, was the representation of the unnamed variables '_'. Initially, we experimented by actually using the character '_' as an attribute value, to represent variables. The performance of the SQL detection queries was satisfactory but we noticed that as the number of variables in a CFD increased, there was a corresponding increase in the detection times (as was already shown in Fig. 3.6(e)). As an alternative, we considered using the null value in a CFD to represent variables. Our SQL detection queries were affected since the term



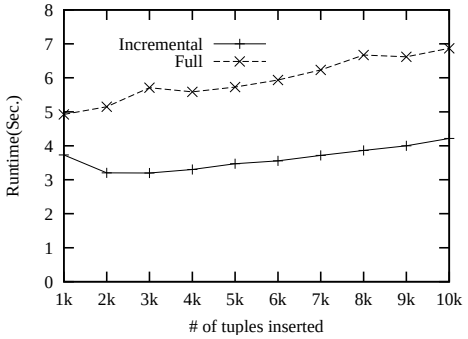
(a) Deleting from 10 to 100 tuples



(b) Deleting from 1,000 to 10,000 tuples



(c) Inserting from 10 to 100 tuples



(d) Inserting from 1,000 to 10,000 tuples

Figure 3.7: Experimental results

($t_p[X_i]$ = '_') was now changed to ($t_p[X_i]$ **is** null). Performance-wise, there was a 10%-20% improvement on detection times. Although an increase on the number of variables in a CFD still resulted in an increase on detection times, detection times scaled much more gracefully with null than when the '_' character was used.

3.3.3 Incremental CFD Detection

For our third set of experiments, we used a relation with SZ 100K, and NOISE 5%. In terms of the CFD, TABSZ was 500 and NUMATTRs was 3.

– **Single tuple deletions:** In this experiment, we consider sets of tuples ranging from 10 to 100 tuples, in 10 tuple increments. For each set, we delete its tuples one-by-one, and after each deletion we use incremental detection to discover violations. So, for the set of 10

tuples, we call incremental detection 10 times, once for each deleted tuple. In Fig. 3.7(a), we report the cumulative time of incremental detection, after all the tuples in the set have been deleted. So in the case of deleting 10 tuples, the reported time is the sum of running 10 times the incremental detection. At the same tine, we also report the time for full (non-incremental) detection, where full detection is performed only *once*, after all the tuples in the set have been deleted. So, while incremental detection is called after each tuple deletion, full detection is only called at the end of deleting all tuples. Note in the figure that the line for incremental detection falls on the x-axis and is not visible. On the other hand, full detection is an order of a mmagnitudeslower, proving clearly the gains of the former method over the latter.

– **Batch tuple deletions:** We now consider deleting sets of tuples ranging from 1,000 to 10,000 tuples, in 1,000 increments. For each set, we perform batch deletion, use incremental detection, and measure its running time. Similarly, after each batch deletion we also use full detection, and measure its running time also. In Fig. 3.7(b), we report the measured times, for each set. As expected, the more tuples we delete, the faster full detection becomes since it has to consider less tuples after the deletion. At the same time, the larger the batch of tuples we delete, the more time incremental detection takes. This is because in Step 2 of the incremental detection during deletion, we have to consider an increasing number of tuples to incrementally detect. The crossing point is around 9,000 tuples. Given our initial relation of 100K tuples, even if we delete around 10% of this relation, a considerable portion by any standard, incremental detection is still a better choice than doing a full detection. In general one can achieve optimal detection times through a simple algorithm that considers the size of the base relation and the number of tuples to be deleted and it chooses between executing an incremental or a full detection.

– **Single tuple insertions:** Similar to single tuple deletions, we consider inserting sets of tuples ranging from 10 to 100 tuples, in 10 tuple increments. We also used the same experimental strategy as single tuple deletions by measuring the cumulative incremental detection time, for all the tuples in the set, versus the full detection time after all the tuples have been deleted. Figure 3.7(c) shows that for any reasonable number of insertions, incremental detection does better than periodically doing full detection. In the worst case, incremental detection is twice as fast as full detection, while for a few tuples it is almost an

order of magnitude faster.

– **Batch tuple insertions:** Similar to batch tuple deletions, we consider batch tuple insertions. As expected, Fig. 3.7(d) shows that as the number of tuples inserted increases, so does the time to execute a full detection. A similar increase is noticed in the multi-step incremental detection and unlike batch deletions, there is no crossing point here even when a considerable number of new tuples are inserted. So, incremental detection is a clear winner, for batch tuple insertions.

Chapter 4

Repairing the Inconsistent Data

Inconsistencies, errors and conflicts in a database often emerge as violations of integrity constraints [ABC99, RD00]. We have seen that CFDs are capable of capturing more *inconsistencies* as constraint violations than traditional FDs and how to use CFDs to detect violations in a database instance. An important problem for data cleaning is how to make the data *consistent*: given a dirty database D, we want to minimally *edit* the data in D such that it satisfies certain constraints. In other words, we want to find a *repair* of D, i.e. a database Repr that satisfies the constraints and is as close to the original D as possible. This is the data cleaning approach that US national statistical agencies, among others, have been practicing for decades [FH76, Win04]. Manually editing the data is unrealistic when the database D is large. Indeed, manually cleaning a set of census data could easily take months by dozens of clerks [Win04]. This highlights the need for automated methods to find a repair of D.

In practice one also wants *incremental* methods to improve the consistency of the data: given a clean database D that satisfies a set Σ of constraints, and updates ΔD on the database D, it is to find a repair ΔD_{Repr} of ΔD such that $D \oplus \Delta D_{\mathsf{Repr}}$ satisfies Σ (we use $\oplus$ to denote the application of updates). This is often advantageous to *batch* methods that compute a repair Repr of $D \oplus \Delta D$ starting from scratch instead of finding a typically much smaller ΔD_{Repr}.

4.1 Data Cleaning Sub-framework

Once the errors and conflicts in a database are detected as violations of CFDs, the next question is how to resolve these violations and hence improve data consistency? Moreover, as there may exist (possibly infinitely) many repairs, which candidate repair should be chosen? Furthermore, how can one tell whether a repair is accurate or not? In this section we answer these questions, state the problems we will tackle, and present an overview of the data-cleaning sub-framework.

4.1.1 Violations and Repair Operations

We first formalize the notion of violations, which helps us decide how "dirty" a data tuple is. We then discuss edit operations to resolve the violations.

Consider a database D and a set Σ of CFDs. For each tuple t in D, the *number of violations* incurred by t, denoted by $\mathsf{vio}(t)$, is computed as follows. Initially $\mathsf{vio}(t)$ is set to 0.

(1) For each CFD $\phi = (R : X \rightarrow A,\ t_p)$ in Σ, if $t[X] \asymp t_p[X]$ but $t[A] \not\asymp t_p[A]$, we say that t *violates* ϕ, and increase $\mathsf{vio}(t)$ by 1. This may occur when $t_p[A] \neq$ '_', i.e. $t_p[A]$ is a constant.

(2) For each CFD $\phi = (R : X \rightarrow A,\ t_p)$ in Σ, if $t[X] \asymp t_p[X]$ and $t_p[A] =$ '_', then for *each* tuple t' in D such that $t[X] = t'[X] \asymp t_p[X]$ but $t[A] \neq t'[A]$, we say that t *violates* ϕ *with* t', and add 1 to $\mathsf{vio}(t)$. Note that if $t_p[A] \neq$ '_' the violation is already covered by case (1) above.

For a subset C of D, the number of violations in C is defined to be the sum of $\mathsf{vio}(t)$ for all t in C, denoted by $\mathsf{vio}(C)$.

A repair Repr of a database D *w.r.t.* a set Σ of CFDs is a database that (i) satisfies Σ, i.e. $\mathsf{Repr} \models \Sigma$, and (ii) is obtained from D by means of a set of *repair operations*.

We consider *attribute value modifications* as repair operations, along the same lines as [BFFR05, FPL+01, LB07a, Wij05]. Note that tuple insertions do not lead to repairs when CFDs (or FDs) are concerned, and that tuple deletions can be mimicked by attribute value modifications.

When we modify the A-attribute of a tuple t in the database D, we either draw its value

from $\mathsf{adom}(A, D)$, i.e. the set of A-attribute values occurring in D, or use the special value null when necessary. That is, we do *not invent* new values. We pick null if the value of an attribute is *unknown* or *uncertain*. To simplify the discussion we assume that one can keep track of a given tuple t in D during the repair process despite that the value of t may change (this can be achieved by e.g. using a temporary unique tuple id).

Attribute value modifications are sufficient to resolve CFD violations: If a tuple t violates a CFD $\phi = (R : X \rightarrow A,\ t_p)$ (case 1 above), we *resolve the* CFD *violation* by either modifying the values of the $\mathsf{RHS}(\phi)$ attribute such that $t[A] \asymp t_p[A]$, or changing the values of some $\mathsf{LHS}(\phi)$ attributes such that $t[X] \not\asymp t_p[X]$. If t violates ϕ with another tuple t' (case 2 above), we either modify $t[A]$ (resp. $t'[A]$) such that $t[A] = t'[A]$, or change $t[X]$ (resp. $t'[X]$) such that $t[X] \not\asymp t_p[X]$ (resp. $t'[X] \not\asymp t_p[X]$) or $t[X] \neq t'[X]$.

Remarks. (1) We adopt the *simple* semantics of the SQL standard [Int03] for null: $t_1[X] = t_2[X]$ evaluates to true if *either one* of them contains null. (2) In contrast, when matching a data tuple t and a pattern tuple t_p, $t[X] \asymp t_p[X]$ is false if $t[X]$ contains null, i.e. CFDs only apply to those tuples that precisely match a pattern tuple, which does not contain null. (3) In case some attributes are non-nullable, we use SET DEFAULT to reset attributes values to their default value. The semantics of the matching operator is redefined accordingly. For convenience, we assume that all attributes are nullable. (4) A tuple can be "deleted" via value modifications by setting null to all of its attributes.

4.1.2 Cost Model

As a violation may be resolved in more than one way, an immediate question is which one to choose? One might be tempted to pick the one that incurs least repair operations. While such a repair is close to the original data, it may not be accurate.

We would like to make the decision based on both the accuracy of the attribute values to be modified, and the "closeness" of the new value to the original value. We assume that a *weight* in the range $[0, 1]$ is associated with each attribute A of each tuple t in the dataset D, denoted by $w(t, A)$ (see the wt rows in Fig. 4.1). The weight reflects the confidence of the *accuracy* placed by the user in the *attribute* $t[A]$, and can be propagated via data provenance analysis in data transformations. Given this, we extend the cost model of [BFFR05] to provide a guidance for how to choose a repair.

	NAME	CNT	CITY	STR	ZIP	CC	AC	PN
t_1:	Eric	US	CHI	Tree Ave.	10112	1	215	1111111
wt	(0.5)	(0.9)	(0.5)	(0.5)	(0.2)	(0.8)	(0.8)	(0.8)
t_2:	Luke	US	PHI	Elm Str.	19117	1	215	2222222
wt	(0.5)	(0.9)	(0.2)	(0.9)	(0.6)	(0.7)	(0.6)	(0.6)
t_3:	John	US	NYC	East Str.	19117	1	212	3333333
wt	(0.5)	(0.9)	(0.3)	(0.9)	(0.2)	(0.7)	(0.6)	(0.6)
t_4:	Dan	US	CHI	Oak Ave.	19114	44	215	4444444
wt	(0.5)	(0.9)	(0.3)	(0.5)	(0.5)	(0.7)	(0.4)	(0.3)
t_5:	Gary	US	NYC	South Ave.	19255	1	212	5555555
wt	(0.5)	(0.9)	(0.3)	(0.5)	(0.5)	(0.6)	(0.5)	(0.5)
t_6:	Mark	US	PHI	West Ave.	19112	1	215	6666666
wt	(0.5)	(0.9)	(0.3)	(0.5)	(0.5)	(0.6)	(0.4)	(0.4)

(a) Example customer data

$T_2 =$

CNT	ZIP	CITY
_	_	_
US	10112	NYC
US	19114	PHI
US	19255	PHI

(b) $\varphi_2 = ([\text{CNT}, \text{ZIP}] \rightarrow [\text{CITY}],\ T_2)$

$T_4 =$

CC	AC	CITY
44	_	_
1	212	NYC
1	215	PHI

(c) $\varphi_4 = ([\text{CC}, \text{AC}] \rightarrow [\text{CITY}],\ T_4)$

$T_5 =$

CC	AC	CNT
_	_	_
44	_	UK
1	215	US

(d) $\varphi_5 = ([\text{CC}, \text{AC}] \rightarrow [\text{CNT}],\ T_5)$

Figure 4.1: Example data and CFDs

For two values v, v' in the same domain, we assume that a *distance function* $\text{dis}(v, v')$ is in place, with lower values indicating greater similarity. In our implementation, we simply adopt the Damerau-Levenshtein (DL) metric [GFS+01], which is defined as the minimum

number of single-character insertions, deletions and substitutions required to transform v to v'.

The cost of changing the value of an attribute $t[A]$ from v to v' is defined to be:

$$\mathsf{cost}(v, v') = w(t, A) \cdot \mathsf{dis}(v, v') / \mathsf{max}(|v|, |v'|),$$

Intuitively, the more accurate the original $t[A]$ value v is and more distant the new value v' is from v, the higher the cost of this change. We use $\mathsf{dis}(v, v')/\mathsf{max}(|v|, |v'|)$ to measure the similarity of v and v' to ensure that longer strings with 1-character difference are closer than shorter strings with 1-character difference.

The cost of changing the value of an R-tuple t to t' is the sum of $\mathsf{cost}(t[A], t'[A])$ for each $A \in \mathsf{attr}(R)$ for which the value of $t[A]$ is modified. The cost of a repair Repr of D, denoted $\mathsf{cost}(\mathsf{Repr}, D)$ is the sum of the costs of modifying tuples in D.

Example 4.1: Consider another example instance of the customer relation, the CFDs φ_2 and φ_4 introduced in Example 3.1, and a new CFD φ_5 modified from CFD φ_1, as shown in Fig. 4.1. CFD φ_5 asserts that for any two customer tuples, if they have the same country code and area code, then they must have the same country name, and moreover, it specifies that for all tuples with country code `44`, the country name must be `UK`, and similarly for all tuples with country code `1` and area code `212` or `215`, the country name must be `US`.

Obviously, tuple t_4 violates CFDs φ_5 since $t_4[\mathsf{CC}] = \texttt{44}$, but $t_4[\mathsf{CNT}] \neq \texttt{UK}$; it also violates φ_2: although $t_4[\mathsf{CNT}] = \texttt{US}$ and $t_4[\mathsf{ZIP}] = \texttt{19114}$, $t_4[\mathsf{CITY}] \neq \texttt{PHI}$.

There are at least two alternative methods to resolve the violations by changing
(1) $t_4[\mathsf{CNT}]$ to `UK`, or
(2) $t_4[\mathsf{CC}]$ to `1` and $t_4[\mathsf{CITY}]$ to `PHI`.

The costs of these repairs are 1/2 * 0.9 = 0.45 and 2/2 * 0.1 + 1/3 * 0.3 = 0.2, respectively, in favor of option (2). Indeed, although option (2) involves more editings than option (1), it may be more reasonable since the weights of $t_4[\mathsf{CC}, \mathsf{CITY}]$ indicate that these attributes are less trustable and thus are good candidates to change. □

Remarks. (1) Although the cost model incorporates the weight information, our cleaning algorithms to be given shortly do not necessarily rely on this. In the absence of the weight information, our algorithms set $w(t, A)$ to 1 for each attribute A of each tuple t. In this case our algorithms use the number of violations $\mathsf{vio}(t)$ to guide repairing process, and our

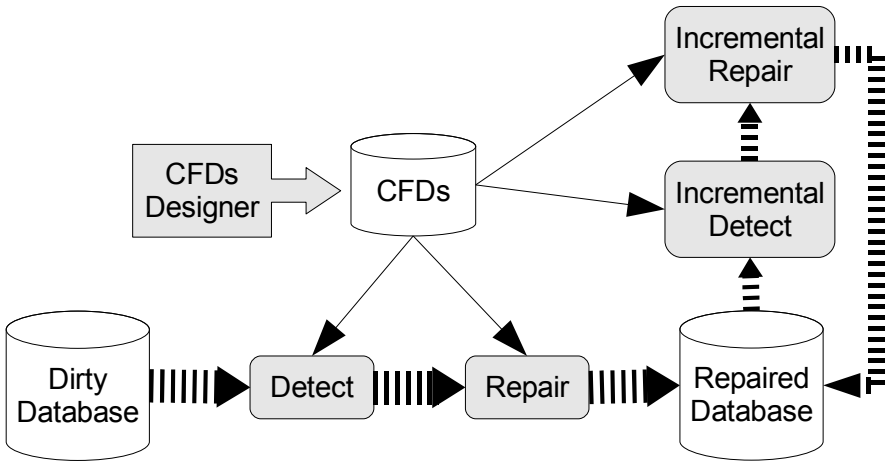


Figure 4.2: Data cleaning sub-framework

experimental results show that the algorithms work well even when the weight information is not available. (2) Other similarity metrics (see, e.g. [CRF03]) can also be used instead of the DL metric in our model.

4.1.3 An Overview of Data Cleaning Sub-framework

The *repairing* problem is stated as follows: given a set Σ of CFDs over a schema R and a database instance D of R, it is to compute a repair Repr of D such that $\mathsf{Repr} \models \Sigma$ and $\mathsf{cost}(\mathsf{Repr}, D)$ is minimum. That is, we want *automated* methods to find a repair *consistent w.r.t.* Σ by modifying D. Intuitively, the smaller $\mathsf{cost}(\mathsf{Repr}, D)$ is, the more accurate and closer to the original data Repr is.

We also study the *incremental repairing problem*: suppose that the database D is consistent, i.e. $D \models \Sigma$. Given updates ΔD to D, we want to find a repair ΔD_{Repr} of ΔD such that $D \oplus \Delta D_{\mathsf{Repr}} \models \Sigma$ and $\mathsf{cost}(\Delta D_{\mathsf{Repr}}, \Delta D)$ is minimum. Since small ΔD often incurs a small number of CFD violations, and because D is clean and thus should not be updated, it is more reasonable and more efficient to compute ΔD_{Repr} than computing a repair Repr of $D \oplus \Delta D$ starting from scratch. We consider *group updates*: ΔD is a set of tuples to be inserted or deleted. For any deletions ΔD, the tuples can be simply removed from D without causing any CFD violation. Thus we need only to consider tuple insertion.

Together with the modeling and detection modules presented in the last chapter, we

develop a sub-framework for data cleaning as shown in Fig. 4.2. The framework consists of five modules.

1. The CFDs designer provides an interface for domain experts to input the CFDs and load the tableaux. Moreover, the static analyses (CFDs consistency checking, computing a minimal cover through CFDs inference system) developed in [BFG+07] could be incorporated to help users to design the CFDs. Note that the CFDs themselves are also stored in the database and standard index can created for pattern tableaux to accelerate the data cleaning process.

2. The detecting and repairing module take as input a database D and a set Σ of CFDs. It *automatically* finds a repair Repr.

3. The incremental detecting and repairing module takes updates ΔD as additional input, and *automatically* finds repair ΔD_{Repr}.

In the next two sections, we present algorithms and methods for supporting the (incremental) repairing modules.

4.2 An Algorithm for Finding Repairs

We now present an algorithm for the repairing module, which *automatically* finds a candidate repair for an inconsistent database.

It is nontrivial to find a quality repair. As shown in [BFFR05], the repairing problem is already NP-complete for standard FDs even when the relational schema and FDs are fixed (i.e. the intractability is the data complexity). We show that for CFDs the problem remains NP-complete, i.e. CFDs do not add to the complexity of this problem.

Corollary 4.2.1: *The repairing problem for* CFD*s is* NP*-complete, even for a fixed database schema and a fixed set of* CFD*s.* □

Proof: Since FDs are a special case of CFDs, the NP-hardness of the CFD-repairing problem follows immediately from the NP-hardness of the FD-repairing problem which is shown to be NP-complete in [BFFR05].

Membership in NP is shown as follows. Given a database D, a (PTIME-computable) cost function cost, a set Σ of CFDs and a constant C we first guess a database instance Repr

consisting of as many tuples as D and then verify in PTIME whether Repr is indeed a repair. That is, we need to check whether (i) $\mathsf{cost}(\mathsf{Repr}, D) < C$; and (ii) $\mathsf{Repr} \models \Sigma$.

Recall that we assume that each tuple in D has a unique identifier, so to obtain Repr we only need to guess a single tuple for each identifier. Since the attribute values of the guessed tuples come from the active domain of D or is equal to null, we can easily guess such a database Repr.

Because we assume that the cost function is computable in PTIME, property (i) is indeed verifiable in PTIME. The same is true for property (ii). Indeed, one first computes the Cartesian product Repr $\times$ Repr and then test whether each CFD in Σ holds. This last step requires only requires $O(|\mathsf{attr}(R)|)$ time for each tuple in Repr $\times$ Repr. Therefore the total time complexity of verifying (ii) is $O(|\Sigma||\mathsf{Repr}|^2|\mathsf{attr}(R)|)$.

As a result it is indeed PTIME-verifiable whether the guessed database Repr is a repair. Therefore, we may conclude that the CFD-repairing problem is in NP. □

This tells us that practical automated methods for this problem have to be heuristic. Worse, although CFDs do not increase the worst-case complexity, previous methods for repairing FDs no longer work on CFDs. Indeed, while it suffices to resolve FD violations by only editing values of attributes in the RHS of FDs [BFFR05], this strategy may not terminate on CFDs, as shown by the next example.

Example 4.2: Recall the customer instance in Fig. 4.1. Tuple t_5 violates CFD φ_2 since $t_5[\mathsf{CNT}] = \mathtt{US}$ and $t_5[\mathsf{ZIP}] = \mathtt{19255}$, but $t_5[\mathsf{CITY}] \neq \mathtt{PHI}$.

While this violation can be resolved by changing the value of the $\mathsf{RHS}(\varphi_2)$ attribute, i.e., $t_5[\mathsf{CITY}]$, from NYC to PHI, this introduces a violation of φ_4. This can no longer be resolved by changing the value of the $\mathsf{RHS}(\varphi_4)$ attribute $t_5[\mathsf{CITY}]$ back to NYC as suggested by φ_4, since otherwise we are back to the original t_5, have to resolve the violation of φ_2 again, and end up with an infinite process. □

To cope with this we present a repair algorithm, BATCHREPAIR, which is a nontrivial extension of the algorithm for FDs proposed in [BFFR05]. It extends the notion of equivalence classes of [BFFR05], and it guarantees to terminate and finds a repair *w.r.t.* CFDs.

4.2.1 Resolving CFD Violations

We first revise the notion of equivalence classes explored in [BFFR05], and then present our strategy for repairing CFDs.

Equivalence classes. An *equivalence class* consists of pairs of the form (t,A), where t identifies a tuple in which A is an attribute. In a database D, each tuple t and each attribute A in t have an associated equivalence class, denoted by $\mathsf{eq}(t,A)$.

In a repair we will assign a unique *target value* to each equivalence class E, denoted by $\mathsf{targ}(E)$. That is, for all $(t,A) \in E$, $t[A]$ has the same value $\mathsf{targ}(E)$. The target value $\mathsf{targ}(E)$ can be either '_', a constant a, or null, where '_' indicates that $\mathsf{targ}(E)$ is not yet fixed, and null means that $\mathsf{targ}(E)$ is uncertain due to conflict. To resolve CFD violations we may "upgrade" $\mathsf{targ}(E)$ from '_' to a constant a, or from a to null, but not the other way around. In particular, we *do not* change $\mathsf{targ}(E)$ from one constant to another.

Intuitively, we resolve CFD violations by *merging* or *modifying* the target values of equivalence classes. Consider a CFD $\phi = (R : X \to A,\ t_p)$. For any pair of tuples t_1 and t_2 in D, if $t_1[X] = t_2[X] \asymp t_p[X]$, then (t_1,A) and (t_2,A) should belong to the *same* equivalence class and eventually, $t_p[A] \asymp \mathsf{targ}(E)$. If $(t_1,A) \neq (t_2,A)$, we may be able to resolve the violation by merging $\mathsf{eq}(t_1,A)$ and $\mathsf{eq}(t_2,A)$ into one. By using equivalence classes, we separate the decision of which attribute values should be equal from the decision of what value should be assigned to the equivalence class. We defer the assignment of $\mathsf{targ}(E)$ as much as possible to reduce poor local decisions, such as changing the value of $t_5[\mathsf{CITY}]$ in Example 4.2.

We use $\mathcal{E}$ to keep track of the current set of equivalence classes in a database D. Initially, $\mathcal{E}$ consists of $\mathsf{eq}(t,A)$ for all tuples t in D and all attribute A in t, where $\mathsf{eq}(t,A)$ starts with a single pair (t,A), with $\mathsf{targ}(\mathsf{eq}(t,A)) =$ _.

Procedure CFD-RESOLVE. Leveraging equivalence classes, we present the main idea of our strategy for resolving CFD violations, which is done by procedure CFD-RESOLVE, a key component of algorithm BATCHREPAIR.

Procedure CFD-RESOLVE takes as input a pair (t,A) and a CFD $\varphi = (R : X \to A, t_p)$, where t violates φ. Recall from Section 4.1.1 that t may violate φ if $t[X] \asymp t_p[X]$ and in addition, either (1) $t[A] \not\asymp t_p[A]$ and $t_p[A]$ is a constant a; or (2) there exists another tuple t' such that $t'[X] = t[X]$ but $t'[A] \neq t[A]$, where $t_p[A] =$ _. The procedure resolves the violation

as follows.

(1) $t[A] \not\asymp t_p[A]$ and $t_p[A] = a$. There are two cases to consider.

(1.1) If $\mathsf{targ}(\mathsf{eq}(t,A))$ = '_', i.e. the target value of $\mathsf{eq}(t,A)$ is not yet fixed, we resolve this by simply letting $\mathsf{targ}(\mathsf{eq}(t,A)) := a$.

(1.2) Otherwise $\mathsf{targ}(\mathsf{eq}(t,A))$ is either a distinct constant b, or null for which we know that the value cannot be made certain. In this case we have to change the value of some $\mathsf{LHS}(\varphi)$ attribute of t, a situation that does not arise when repairing traditional FDs.

More specifically, we look at each attribute $B_i \in X$ such that $\mathsf{targ}(\mathsf{eq}(t,B_i))$ is '_', i.e. not yet fixed. If no such B_i exists, we cannot resolve the conflict with a certain value. Thus we pick B_i such that the sum of weights of attributes in $\mathsf{eq}(t,B_i)$ is minimal, and change $\mathsf{targ}(\mathsf{eq}(t,B_i))$ to null. If there exists B_i with $\mathsf{targ}(\mathsf{eq}(t,B_i)) = \_$, we pick such a B_i and a value v such that $\mathsf{cost}(\mathsf{eq}(t[B_i]),v)$ is minimum, and let $\mathsf{targ}(\mathsf{eq}(t,B_i)) := v$. The value v is picked by a procedure FINDV, which we shall discuss shortly, along with the definition of $\mathsf{cost}(\mathsf{eq}(t[B_i]),v)$.

Example 4.3: Consider again the setting of Example 4.1, tuple t_1 violates CFD φ_2 since $t_1[\mathsf{CNT}] = \mathtt{US}$ and $t_1[\mathsf{ZIP}] = \mathtt{10112}$, but $t_1[\mathsf{CITY}] \neq \mathtt{NYC}$; it also violates φ_4: although $t_1[\mathsf{CC}] = \mathtt{1}$ and $t_1[\mathsf{AC}] = \mathtt{215}$, $t_1[\mathsf{CITY}] \neq \mathtt{PHI}$.

Suppose that we want to resolve the violation of φ_2 caused by tuple t_1. If $\mathsf{targ}(\mathsf{eq}(t_1,\mathsf{CITY}))$ is '_', we can resolve this by simply letting them to be NYC. However, if this target value was already set to PHI when, e.g. resolving the violation of φ_4, we can no longer change this target value of the $\mathsf{RHS}(\varphi_2)$ attribute. Hence, we have to change the values of the $\mathsf{LHS}(\varphi_2)$ attributes. Since the weights indicate $t_1[\mathsf{ZIP}]$ is less trustable, now procedure FINDV may set $\mathsf{targ}(\mathsf{eq}(t_1,\mathsf{ZIP}))$ to 19112. If, however, $\mathsf{targ}(\mathsf{eq}(t_1,\mathsf{ZIP}))$ and $\mathsf{targ}(\mathsf{eq}(t_1,\mathsf{CNT}))$ were already given another constants, we set $t_1[\mathsf{ZIP}]$ to null since there is no certain value to resolve the violation. □

(2) t violates φ with another tuple t'. We consider the following cases. Suppose that $\mathsf{targ}(\mathsf{eq}(t,A)) = \eta$ and $\mathsf{targ}(\mathsf{eq}(t',A)) = \eta'$.

(2.1) Neither η nor η' is null, and at least one of them is '_'. In this case the violation is resolved by *merging* $\mathsf{eq}(t,A)$ and $\mathsf{eq}(t',A)$ into one. We remark that this step is identical to

the resolution step for FDs presented in [BFFR05]. In fact this is the *only* operation required to resolve all FD violations. For CFDs, more needs to be done. We let $\mathsf{targ}(\mathsf{eq}(t,A))$ be '_' if both η and and η' are '_'; if one of them is a constant c, we let $\mathsf{targ}(\mathsf{eq}(t,A))$ be c.

(2.2) η' and η' are distinct constants c, c', respectively. Like case (1.2) above, this inconsistency cannot be resolved by changing $\mathsf{RHS}(\varphi)$ attributes, and we have to resolve this by changing some $\mathsf{LHS}(\varphi)$ attribute of either t or t', along the same lines as case (1.2).

(2.3) At least one of η and η' is null. Assume that it is η. Then $t[A]$ will be given null as its value. By the simple semantics of null, $t[A] = \mathsf{targ}(\mathsf{eq}(t',A))$ no matter what value $\mathsf{targ}(\mathsf{eq}(t',A))$ will eventually take. In other words, the violation is already resolved.

Example 4.4: Returning to Example 4.1, tuples t_2 and t_3 violate CFD φ_2 since $t_2[\mathsf{CNT}] = t_3[\mathsf{CNT}]$ and $t_2[\mathsf{ZIP}] = t_3[\mathsf{ZIP}]$, but $t_2[\mathsf{CITY}] \neq t_3[\mathsf{CITY}]$. Suppose that we want to resolve this violation. If the target values of $\mathsf{eq}(t_2, \mathsf{CITY})$ or $\mathsf{eq}(t_3, \mathsf{CITY})$ is '_', and none of them is null, we can resolve the violation by simply merging $\mathsf{eq}(t_2, \mathsf{CITY})$ and $\mathsf{eq}(t_3, \mathsf{CITY})$. In the presence of conflicting target values, e.g. when resolving the violation of φ_4 causes equivalence classes $\mathsf{eq}(t_2, \mathsf{CITY})$ and $\mathsf{eq}(t_3, \mathsf{CITY})$ have distinct constant target values: $\mathsf{targ}(\mathsf{eq}(t_2, \mathsf{CITY}))$ = PHI and $\mathsf{targ}(\mathsf{eq}(t_3, \mathsf{CITY}))$ = NYC, we have to change the target value of the $\mathsf{LHS}(\varphi_2)$ attributes of either t_2 or t_3, i.e. the target value of one of $\mathsf{eq}(t_2, \mathsf{CNT})$, $\mathsf{eq}(t_2, \mathsf{ZIP})$, $\mathsf{eq}(t_3, \mathsf{CNT})$ or $\mathsf{eq}(t_3, \mathsf{ZIP})$. According to the cost, we may set $\mathsf{targ}(\mathsf{eq}(t_3, \mathsf{ZIP}))$ to 10112. □

4.2.2 Batch Repair Algorithm

We now present algorithm BATCHREPAIR. In addition to the set $\mathcal{E}$ of equivalence classes, the algorithm keeps track of violations of CFDs. As we have seen in Example 4.2, a repair may generate *new violations*. Therefore, we maintain for each CFD $\varphi \in \Sigma$ a set $\mathsf{Dirty\_Tuples}(\varphi)$ of tuples that (possibly) violate φ. We update these sets after each resolution of a violation. More precisely, suppose that a violation of φ caused by t is resolved by updating $\mathsf{eq}(t,A)$. Then for each tuple t', if $(t',A) \in \mathsf{eq}(t,A)$, and for each $\psi = (R : X \rightarrow C, t_p)$, if $A \in X \cup \{C\}$, we add t' to $\mathsf{Dirty\_Tuples}(\psi)$. We then remove t from $\mathsf{Dirty\_Tuples}(\varphi)$. In this way Dirty_Tuples always contain all *potentially unresolved* tuples.

Procedure BATCHREPAIR(D,Σ)

Input: A set Σ of CFDs, and a database D.
Output: A repair Repr of D.

1. $\mathcal{E} := \{\{(t,A)\} \mid t \in R, A \in att(R)\}$;
2. **for** each $E \in \mathcal{E}$ **do** /* initializing $\mathsf{targ}(E)$ */
3. $\mathsf{targ}(E) := \_$;
4. Initialize Dirty_Tuples;
5. **while** Dirty_Tuples $\neq \emptyset$
6. $(t,B,v,\varphi) :=$ PICKNEXT();
7. Repr := CFD-RESOLVE(t,B,v,φ);
8. Update Dirty_Tuples;
9. **if** Dirty_Tuples $= \emptyset$ **then**
10. **for** each $E \in \mathcal{E}$ **do**
11. **if** $\mathsf{targ}(E) = \_$ **then** /* instantiating _ */
12. $\mathsf{targ}(E)$:= a constant with the least cost;
13. Update Dirty_Tuples;
14. **for** each $E \in \mathcal{E}$ and each $(t,A) \in E$ **do**
15. $t[A] := \mathsf{targ}(E)$; /* updating D to obtain Repr
16. **return** D.

Figure 4.3: Algorithm BATCHREPAIR

The algorithm is shown in Fig. 4.3. We start with initialization of the set $\mathcal{E}$ of equivalence classes and Dirty_Tuples (lines 1-4). Next, as long as there are dirty tuples (loop on line 5) we greedily look for the "best" next repair. More specifically, the procedure PICK-NEXT loops over each CFD $\varphi \in \Sigma$ and its violating tuple t; it identifies which pair (φ,t) incurs the least cost to repair (line 6). The algorithm then resolves t for φ (line 7), resulting in a modified set of equivalence classes, by invoking procedure CFD-RESOLVE. It then updates the set of dirty tuples (line 8) before finding the next best repair. If no more dirty tuples are unresolved (line 9), then for each equivalence class $E \in \mathcal{E}$ with $\mathsf{targ}(E) = \_$, it

Procedure PICKNEXT()

1. BestCost := ∞;
2. **for** each CFD $\varphi = (R : X \rightarrow A,\ t_p), t \in$ Dirty_Tuples(φ) **do**
3. decide an attribute B in t to update $\mathsf{eq}(t,B)$;
4. $S := \{t' \in R \mid t'[X \cup \{A\} \setminus \{B\}] = t[X \cup \{A\} \setminus \{B\}]\}$;
5. $v :=$ FINDV(t,B,S,φ);
6. **if** $\mathsf{Cost}(t,B,v) <$ BestCost **then**
7. BestFix := (t,B,v,φ); BestCost := $\mathsf{Cost}(t,B,v)$;
8. **return** BestFix;

Figure 4.4: procedure PICKNEXT

finds a constant value with the least cost to instantiate $\mathsf{targ}(E)$ (lines 10-12). That is, *ultimately* all equivalence classes will have either a constant value or null. This instantiation may introduce new violations, and thus Dirty_Tuples should be maintained (line 13). After the loop, we create a repair Repr by editing the original database D by using the target values of equivalence classes (lines 14-15).

The most expensive and elaborate procedure is PICKNEXT (see Fig. 4.4). It finds the next tuple t and CFD φ to be resolved. More specifically, for each CFD φ and its unresolved tuple t, PICKNEXT first decides for which attribute B of t it can update $\mathsf{eq}(t,B)$ to resolve the violation (line 3), following the analysis described in Section 4.2.1. After B is fixed, it finds a set S of tuples that agree with t on all the attributes in φ except B (line 4). The idea is that we may pick a target value v for $\mathsf{eq}(t,B)$ from the B-attribute values of the tuples in S (line 5). It then analyzes the cost of repairing the violation using v (lines 6-7), where $\mathsf{Cost}(t,B,v)$ is defined to be $\sum_{(t',C)\in\mathsf{eq}(t,B)} w(t',C) \cdot \mathsf{dist}(v,t'[C])$. It returns (t,B,v) with the least cost (line 8).

It remains to show how the value v is picked. Given t,B and φ, procedure FINDV (not shown) checks whether $B = A$. If so, v is already determined by either $t_p[A]$ (case (1.1) in Section 4.2.1) or the target values of $\mathsf{eq}(t,A)$ and $\mathsf{eq}(t',A)$ (t' is the tuple with which t violates φ, case (2.1)). Otherwise, i.e. if $B \in \mathsf{LHS}(\varphi)$, it inspects $\mathsf{targ}(\mathsf{eq}(t_1,B))$ for all $t_1 \in S$, and finds v with the least $\mathsf{Cost}(t,B,v)$ such that $v \neq t[B]$. The motivation for picking

v from S is to find a semantically-related value, identified by the pattern $t[X \cup \{A\} \setminus \{B\}]$. If such v does not exist, it lets $v := \mathsf{null}$.

Example 4.5: Continuing with Example 4.3, suppose now that the target value of $\mathsf{eq}(t_1, \mathsf{CITY})$ is `PHI` obtained in repairing φ_4. To resolve the violation of φ_2, we decide to change the target value of $t_1[\mathsf{ZIP}]$. Procedure PICKNEXT finds $S = \{t_2, t_6\}$, i.e. S consists of all tuples t' with `PHI` as the target value of $\mathsf{eq}(t', \mathsf{CITY})$, Now Procedure FINDV attempts to choose v from the target values of $\mathsf{eq}(t', \mathsf{ZIP})$ for $t' \in S$. There are two such values: `19117` and `19112`. It decides to pick `19112` since it incurs least cost. If S were empty or $\mathsf{targ}(\mathsf{eq}(t_1, \mathsf{ZIP}))$ and $\mathsf{targ}(\mathsf{eq}(t_1, \mathsf{CNT}))$ already had constant values, it assigns null to v. □

Upon receiving (t, B, v, φ) from PICKNEXT, procedure CFD-RESOLVE (not shown) in algorithm BATCHREPAIR merges or update the target values of equivalence classes to resolve the violation of φ caused by t, as described in Section 4.2.1.

Correctness. Clearly at each step of algorithm BATCHREPAIR, a CFD violation is resolved. However, each step can also introduce new violations as illustrated in Example 4.2; moreover, a tuple t can appear as a violation multiple times. Nevertheless, BATCHREPAIR always terminates and generates a repair.

Theorem 4.2.2 *Given any database D and any set Σ of* CFD*s,* BATCHREPAIR *terminates and finds a repair* $\mathsf{Repr} \models \Sigma$ *for D.*

Proof: At each step either the total number N of equivalences classes is reduced or the number H of those classes that are assigned a constant or null is increased. Let k be the number of (t, A) pairs in D. Since $N \leq k$ and $H \leq 3 \cdot k$ (the target value of $\mathsf{eq}(t, A)$ can only be '_', a constant, or null), BATCHREPAIR necessarily terminates. Furthermore, since the algorithm proceeds until no more dirty tuples exist, it always finds a repair of D. □

4.3 An Incremental Repairing Algorithm

In this section we present our *incremental algorithm* to improve the consistency of data. Given a clean database D that satisfies a set Σ of CFDs, and a set ΔD of updates on the database D, our algorithm *automatically* finds a repair ΔD_{Repr} of ΔD such that $D \oplus \Delta D_{\mathsf{Repr}}$

satisfies Σ. This is the algorithm underlying the incremental module of our framework shown in Fig 4.2, which tackles the *incremental repairing problem*.

As remarked in Section 4.1.3, it suffices to consider ΔD consisting of insertions only, as deletions never cause any inconsistencies.

One might think that the incremental repairing problem is simpler than its batch (non-incremental) counterpart. Unfortunately it is not the case. Since the repairing problem (see Section 4.1.3) can be seen as an instance of the incremental repairing problem (indeed, just consider the case that $D = \emptyset$), we immediately obtain the following corollary from Theorem 4.2.1.

Corollary 4.3.1: *The incremental repairing problem for* CFD*s is* NP*-complete, even for a fixed schema and a fixed set of* FD*s.* □

Proof: The NP-hardness of the incremental repairing problem follows immediately from Corollary 4.2.1. Indeed, given an instance D and set Σ of CFDs, the non-incremental repairing problem can be solved incrementally by letting $D' = \emptyset$ and $\Delta D' = D$. Membership in NP is shown in exactly the same way as in the proof of Corollary 4.2.1, except that $\Delta D'$ is guessed instead of D'. □

Therefore, we again have to rely on heuristics in the incremental setting. We first develop a heuristic in Section 4.3.1 and then present optimization techniques to improve the algorithm in Section 4.3.2. Finally, we show in Section 4.3.3 that the incremental algorithm in fact provides an alternative method for the repairing problem.

4.3.1 Incremental Algorithm and Local Repairing Problem

Given a set of updates ΔD, Corollary 4.3.1 tells us that it is beyond reach in practice to find an optimal ΔD_{Repr}. Furthermore, we cannot directly apply the algorithm developed for the repairing problem to finding ΔD_{Repr} since we cannot prevent it from updating the clean D. Following the approach commonly used in repairing census data [FH76, Win04], we repair the tuples in ΔD *one at a time* following some ordering O on these tuples. We assume that O is given but will provide various orderings in Section 4.3.2.

Therefore, the key problem is to find, given a clean database D, a tuple t to be inserted into D, and a set Σ of CFDs, a repair Repr_t of t of minimum cost such that $D \cup \{\mathsf{Repr}_t\}$ is a repair. We refer to this as the *local repairing problem*.

Procedure INCREPAIR$(D, \Delta D, \Sigma, O)$

Input: A clean database D, a set Σ of CFDs, a set of updates ΔD, and an ordering O on ΔD.

Output: A repair Repr of $D \oplus \Delta D$ such that $D \subseteq$ Repr.

1. Repr := D;
2. **for** each t in ΔD in the given order O **do**
3. $\quad$ Repr$_t$:= TUPLERESOLVE $(t,$ Repr$, \Sigma)$;
4. $\quad$ Repr := Repr $\cup \{$Repr$_t\}$;
5. **return** Repr.

Figure 4.5: Algorithm INCREPAIR

Algorithm INCREPAIR. The overall driver of our incremental repairing algorithm is presented in Fig. 4.5. Taking as input a database D, a set ΔD of updates, a set Σ of CFDs, and an ordering O on ΔD, it does the following. It first initializes the repair Repr with the current clean database D (line 1). It then invokes a procedure called TUPLERESOLVE (line 3) to repair each tuple t in ΔD according to the given order O (line 2), and adds the local repair Repr$_t$ of t to Repr (line 4) before moving to the next tuple. Once all tuples in ΔD are processed, the final repair is reported (line 5).

The key characteristics of INCREPAIR are (i) that the repair grows at each step, providing in this way more information based on which we can use to clean the next tuple, and (ii) that the data in D is not modified since it is assumed to be clean already.

Algorithm TUPLERESOLVE. The core of the INCREPAIR algorithm is the procedure TUPLERESOLVE that aims to solve the local repairing problem. One might think that the local repairing problem would make our lives easier. However, it is known that the local repairing problem is NP-complete. Moreover, it remains intractable if one considers standard FDs only [CFG$^+$07]. Thus finding the optimal repair Repr$_t$ of t is infeasible in practice. Indeed, the naive approach, namely, enumerating all possible repairs and then selecting the one with the minimal cost, is clearly not an option in case that the number of attributes or the size of the active domains is large.

In light of this intractability, procedure TUPLERESOLVE is based on a *greedy* approach. As shown in Fig. 4.6, it takes as input a single tuple t to be inserted, the current repair Repr,

Procedure TUPLERESOLVE(t, Repr, Σ)

Input: A tuple t to repair, the current repair Repr, and a set Σ of CFDs.
Output: A repair Repr_t of t such that $\mathsf{Repr} \cup \{\mathsf{Repr}_t\} \models \Sigma$.

1. $\mathcal{C} := \emptyset$; $\mathsf{Repr}_t := t$;
2. **while** $\mathsf{attr}(R) \neq \mathcal{C}$ **do**
3. cost := ∞;
4. **for** each $C \in [\mathsf{attr}(R) \setminus \mathcal{C}]_k$ **do**
5. $\mathcal{V} := \{\hat{v} \mid \mathsf{Repr} \cup \{repr_t[C/\hat{v}]\} \models \Sigma(C \cup \mathcal{C})\}$;
6. $\hat{v} := \arg\_\min_{\hat{v} \in \mathcal{V}} \mathsf{costfix}(C, \hat{v})$;
7. **if** $\mathsf{costfix}(C, \hat{v}) <$ cost **then**
8. cost := $\mathsf{costfix}(C, \hat{v})$; BestFix:=$(C, \hat{v})$;
9. $\mathcal{C} := \mathcal{C} \cup C$; $\mathsf{Repr}_t := \mathsf{Repr}_t[C/\hat{t}]$;
10. **return** Repr_t.

Figure 4.6: Algorithm TUPLERESOLVE

and a set Σ of CFDs, and returns a repair Repr_t of t such that $\mathsf{Repr} \cup \{\mathsf{Repr}_t\} \models \Sigma$.

Before we explain TUPLERESOLVE in more detail, we need some notation. For a fixed integer $k > 0$ and a set of attributes $X \subseteq \mathsf{attr}(R)$ we denote by $[X]_k$ the set of all subsets of X of size k. For a tuple t, a set $C \in [X]_k$ and $\bar{v} = (v_1, \ldots, v_k)$, where $v_i \in \mathsf{adom}(D, A_i) \cup \{\mathsf{null}\}$ for each $A_i \in C$, we denote by $t[C/\bar{v}]$ the tuple obtained by replacing $t[A_i]$ by v_i for each $A_i \in C$ and leaving the other attributes unchanged. Finally, for a set Σ of CFDs and a set $X \subseteq \mathsf{attr}(R)$, we denote by $\Sigma(X)$ the set of CFDs in Σ of the form $(R : Y \rightarrow A, t_p)$ with $Y \cup \{A\} \subseteq X$.

We explain how procedure TUPLERESOLVE works in an inductive way. In a nutshell, it greedily finds the "best" sets of attributes of t to modify in order to create a repair. More specifically, for a fixed $k > 0$ it first finds the "best" $C_1 \in [\mathsf{attr}(R)]_k$ (lines 4–9) and attribute values $\hat{v} = (v_1, \ldots, v_k)$ for the attributes in C_1 such that

(i) v_i is in $\mathsf{adom}(\mathsf{Repr}, A_i) \cup \{\mathsf{null}\}$ (line 5);

(ii) $\mathsf{Repr} \cup \{t[C_1/\hat{v}]\}$ satisfies all CFDs in $\Sigma(C_1)$ (line 5); and

(iii) the cost $\mathsf{costfix}(C_1, \hat{v}) = \mathsf{cost}(t, t[C_1/\hat{v}]) \times \mathsf{vio}(t[C_1/\hat{v}])$ is minimal (lines 6–8).

In other words, the predefined parameter k limits the number of possible repairs that we consider. Our experiments show that for $k = 1, 2$ we are already able to obtain good results. We denote the set of all k-tuples $\bar{v}$ satisfying (i) and (ii) by $\mathcal{V}$ (line 5). Once TUPLERESOLVE finds C_1 and $\hat{v}$, C_1 is added to $\mathcal{C}$ and t is replaced by $t_1 = t[C_1/\hat{v}]$ (line 9). Furthermore, TUPLERESOLVE will *never* backtrack and modify t_1 for the attributes in C_1 again.

Suppose that TUPLERESOLVE already selected n best pairwise disjoint sets $C_1, \ldots, C_n$ in $[\mathsf{attr}(R)]_k$ and k-tuples $\hat{v}_1, \ldots, \hat{v}_n$ such that for $t_n = t_{n-1}[C_n/\hat{v}_n]$, we have that $\mathsf{Repr} \cup \{t_n\} \models \Sigma(\mathcal{C})$, where $\mathcal{C} = C_1 \cup \cdots \cup C_{n-1}$. That is, t_n is the current (almost) repair for t. If $\mathsf{attr}(R) = \mathcal{C}$ then clearly t_n is a real repair of t and TUPLERESOLVE will output $\mathsf{Repr}_t = t_n$ (line 2, line 10). Otherwise, TUPLERESOLVE finds the next best set C_{n+1} in $[\mathsf{attr}(R) \setminus \mathcal{C}]_k$ and finds a k-tuple $\hat{v}_{n+1}$ satisfying the same conditions (i)–(iii) as above *except* that the repair $t_{n+1} = t_n[C_{n+1}/\hat{v}_{n+1}]$ must satisfy $\Sigma(C_{n+1} \cup \mathcal{C})$. Again, the set C_{n+1} is then added to $\mathcal{C}$ and the current (almost) repair is set to t_{n+1}. The procedure TUPLERESOLVE keeps selecting such sets of attributes and values until $\mathsf{attr}(R)$ is completely covered.

It is important that $\bar{v}$ is allowed to contain null values (see property (i)). Indeed, this is needed for guaranteeing the existence of k-tuples $\bar{v}$ satisfying property (ii) as the next example illustrates.

Example 4.6: Assume that t_1 in Example 4.1 is an inserted tuple and $k = 1$. Suppose that TUPLERESOLVE already fixed all attributes except CITY. In order for TUPLERESOLVE to repair t_1 it needs to find a tuple $\hat{v} = (v_1)$ for $C = \{\mathsf{CITY}\}$ such that $t_1[C/\hat{v}]$ satisfies both φ_2 and φ_4. As observed in Example 4.3 no such $\hat{v}$ exists when we only consider values in the active domains. Thus the only possible $\hat{v}$ here is (null). In contrast, Example 4.3 shows that C={CITY, ZIP} for $k = 2$, and $\hat{v}$=(PHI, 19112) provides a repair for t_1. □

Correctness. The termination of INCREPAIR follows immediately from the fact that (i) each tuple in ΔD is treated only once; and (ii) each attribute is modified at most once by TUPLERESOLVE. Moreover, TUPLERESOLVE always generates a repair for each tuple in ΔD.

Theorem 4.3.2 *Given a database D, a set Σ of* CFD*s and update ΔD,* INCREPAIR *always terminates and finds a repair ΔD_{Repr} such that $D \oplus \Delta D_{\mathsf{Repr}} \models \Sigma$, regardless of the ordering O.*

4.3.2 Ordering for Processing Tuples and Optimizations

While the ordering O for processing tuples has no impact on the termination of an IncRepair process, it does make a difference when it comes to repairing performance and the accuracy of the repair. We next study various orderings, based on which we develop (and experiment with) variants of the IncRepair algorithm.

Theorem 4.2.1 tells us that it is beyond reach in practice to find an ordering that leads to an optimal repair. Thus we propose and experiment with the following orderings.

Linear-scan ordering. A naive approach is to adopt an arbitrary linear-scan order for O, with the benefit that it incurs no extra cost. We refer to IncRepair based on this as L-IncRepair.

A greedy algorithm based on violations. This algorithm, referred to as V-IncRepair, is based on the *number of violations* $\mathsf{vio}(t)$ of each tuple t, which is defined in Section 4.1.1. A tuple $t \in D$ might cause multiple violations of constraints in Σ. Intuitively, the less $\mathsf{vio}(t)$ is, the more accurate t is and the less costly to repair it. Algorithm V-IncRepair repairs tuples in the *increasing* order of $\mathsf{vio}(t)$ so that accurate tuples are included in Repr early, and based on them we resolve violations of "less accurate" tuples.

A greedy algorithm based on weights. Another approach is based on the weight $\mathsf{wt}(t)$ of a tuple t (recall the definition of $\mathsf{wt}(t)$ from Section 4.1.2). Intuitively, the larger $\mathsf{wt}(t)$ is, the more accurate t is. We develop a variant of IncRepair, referred to as W-IncRepair, which processes tuples based on the *decreasing* order of $\mathsf{wt}(t)$ to reduce the cost and improve the quality of repairs found.

We next present optimizations adopted by our algorithm.

Optimization. The main computational cost of IncRepair lies in the procedure TupleResolve. Indeed, there one needs to (i) consider all possible subsets C of attributes of size k; (ii) for each such C compute the set $\mathcal{V}$ consisting of all possible k-tuples $\bar{v}$ on the attributes in C that satisfy the relevant CFDs; and (iii) obtain from $\mathcal{V}$ the tuple $\hat{v}$ that has minimal cost with $t[C]$ (Fig 4.6, lines 5–6). To do these tasks efficiently we leverage the use of indices.

LHS-indices. For each CFD $(R : X \to A,\ t_p)$ in Σ we build an index I for the embedded FD $X \to A$. The index consists of pairs $\langle \mathsf{key}, \mathsf{it} \rangle$ where key uniquely identifies item it in I and

is constructed as follows: if $t_p[A] = a$, then we simply add $\langle t_p[X], a\rangle$ to I; if $t_p[A] = \_$, then we add for each tuple $t' \in \mathsf{Repr}$ such that $t'[X] \asymp t_p[X]$ the pair $\langle t''[X], t''[A]\rangle$ to I. Observe that because Repr is clean, such keys provide indeed a unique identifier.

Now, given a tuple t' and a fixed set of attributes C, we can efficiently determine whether or not a candidate repair $t'' = t'[C/\bar{v}]$ violates a CFD $(R : X \to A,\ t_p)$ in $\Sigma(C \cup C)$ by (i) searching the index for φ using $t''[X]$ as key; and (ii) testing whether $t''[A]$ matches the returned item. Doing this for all CFDs allows us to compute the number of violations of a candidate repair efficiently.

Finally, these indices are dynamically updated when repairs are added to Repr using standard update mechanisms.

Cost-based indices. We arrange the values of $\mathsf{adom}(\mathsf{Repr}, A)$ for each attribute A in a tree structure, by using a hierarchical agglomerative clustering method [HK06]. In the tree, "similar" values are grouped together based on the DL metric. Recall that the DL metric between two values is defined as the minimum number of single-character insertions, deletions and substitutions required to transform one to another. Suppose for the moment that we are considering a single attribute A only and want to range over $\mathsf{adom}(\mathsf{Repr}, A)$ such that values are considered in decreasing similarity to a given attribute value $t[A]$. We then simply iterate over $\mathsf{adom}(\mathsf{Repr}, A)$ by first searching for $t[A]$, starting from the root, and then moving to its child cluster that is closest to $t[A]$ in terms of the DL metric. This process then continues until we find a value modification for $t[A]$ that satisfies the requirements given in TUPLERESOLVE. If no suitable candidate can be found, we simply use null. In case of multiple attributes (recall that TUPLERESOLVE tries to find k-tuples), we range over the individual trees in a nested way until a suitable candidate tuple is found. Again, we introduce null whenever no suitable attribute value can be found.

4.3.3 Applying INCREPAIR in the Non-incremental Setting

Algorithm INCREPAIR can also be used in the non-incremental setting. Indeed, given a dirty database D' one can first extract a maximal consistent set of tuples D from D' and then simply apply INCREPAIR to D and $\Delta D = D' \setminus D$. However, computing such a maximal set of tuples might be too hard in practice: [CFG+07] has shown that it is NP-hard to find, given a dataset D' and a set Σ of CFDs, a maximal subset C of D' such that $C \models \Sigma$.

Greedy algorithms do provide some approximation guarantees [BH92] for finding such a set C. However, unless for each CFD $\varphi \in \Sigma$ the number of tuples that violate φ with another tuple is bounded by a small constant, the approximation factor grows with the size of the database [HR94]. A simpler approach is to compute the set C' of tuples that do not violate *any* constraint in Σ. This clearly does not gives us a maximal set of tuples but as shown in the last chapter it can be efficiently computed using SQL queries. Moreover, in practice one can often expect this set to be fairly large. Indeed, some studies have found common error rates of 1%–5% of real-world data in enterprises [Red98].

4.4 Experimental Study: Repairing CFD Violations

In this section, we present an experimental study of our repairing algorithms. We investigate the repair quality, scalability, and sensitivity to error rate and types of violations for both BATCHREPAIR and INCREPAIR.

4.4.1 Experimental Setting

Our experiments were conducted on an Apple Xserve with 2.3GHz PowerPC dual CPU and 4GB of memory; of those, at most 2GB could be used by our system. We used a commercial DBMS on the same machine.

Data and constraints. Our experiments used an extension of the relation shown in Fig. 4.1. Specifically, its schema models a company's sales records and includes 4 additional attributes, namely, the country of the customer CTY, the tax rate of the item VAT, the title TT and quantity of the item QTT. To populate this table, we scraped data from AMAZON and other websites as seed, and generated datasets of various sizes, ranging from 10k to 300k tuples. The generation process is explained later.

Our set Σ consists of 7 CFDs: 5 taken from Fig. 4.1 and Fig. 3.2, together with two new cyclic CFDs.

We included 300–5,000 tuples in the pattern tableaux of these CFDs, enforcing patterns of semantically related values which we identified through analyzing the real data. Note that the set of constraints is fairly large since each pattern tuple is in fact a constraint.

We first populated the table such that the initial datasets are consistent with all the CFDs in Σ. We refer to this "correct" data as D_{opt}. We then introduced noise to attributes in D_{opt} such that each "dirty" tuple violates at least one or more CFDs. To add noise to an attribute, we randomly changed it either to a new value which is close in terms of DL metric (distance between 1 and 6) or to an existing value taken from another tuple. This is reasonable as in real life noise is often due to typos or wrong values in the domain. Such "dirty" dataset is referred to as D. We used a parameter ρ ranging from 1% to 10% for the noise rate.

Moreover, in accordance to the cost model defined in Section 4.1.2 we set weights to the attributes of tuples in D in the following way. Suppose that t is a tuple in D, then we say that A is a "clean" attribute for t if the corresponding tuple t' in D_{opt} agrees with t on attribute A; otherwise we call A "dirty" for t. For dirty attributes in t, we randomly assign a weight $w(t,A)$ in $[0,a]$; for clean attributes we randomly select a weight $w(t,A)$ in $[b,1]$. This is based on the assumption that a clean attribute usually has a slightly higher weight than a dirty attribute. In the experiments, we set $a = 0.6$ and $b = 0.5$. We also studied the case when no weight information was available, by setting the weights to 1 for all attributes.

Algorithms. We have implemented prototypes of BATCHREPAIR and all three variants of INCREPAIR, i.e. L-INCREPAIR, V-INCREPAIR and W-INCREPAIR, all in Java. In the experiments we used INCREPAIR to repair the entire data set, as described in Section 4.3.3, except in one occasion (Fig. 4.8(b)). That is, L-INCREPAIR, V-INCREPAIR and W-INCREPAIR were applied to non-incremental setting except for Fig. 4.8(b).

Measuring repair quality. There is no benchmark algorithm available for repairing CFDs. While each repair Repr of the database D found by our algorithms satisfies all the CFDs (this follows from the correctness of our algorithms), it still may contain two types of errors: (a) the noises that are not fixed, and (b) the new noises introduced in the repairing process. Although it is important to distinguish these two types of errors, the metrics used in previous data cleaning work often considers the first type of errors while ignoring the second type. For example, [BFFR05] measures *the percentage of error corrected*, which does not distinguish these two types of errors.

To measure these two types of errors, we used the notions of *Precision* and *Recall*, which are widely used in information retrieval and many other areas. *Precision* is the ratio of the number of correctly repaired noises to the number of changes made by the repairing

algorithm. It measures the repair correctness. *Recall* is the ratio of the number of correctly repaired noises to the total number of noises. It measures repair completeness. For a dirty dataset D and a Repr found by our algorithms, we compute the number of noises by $\mathsf{dif}(D, D_{\mathsf{opt}})$ (recall that we know D_{opt}). The number of changes made by the repairing algorithm is $\mathsf{dif}(D, \mathsf{Repr})$ and the number of noises correctly repaired is $\mathsf{dif}(D, \mathsf{Repr}) - \mathsf{dif}(D_{\mathsf{opt}}, \mathsf{Repr})$. Note that our algorithm may change some values to null. If such a value before the change is correct, we count the null as an error; otherwise, we treat it as a correction.

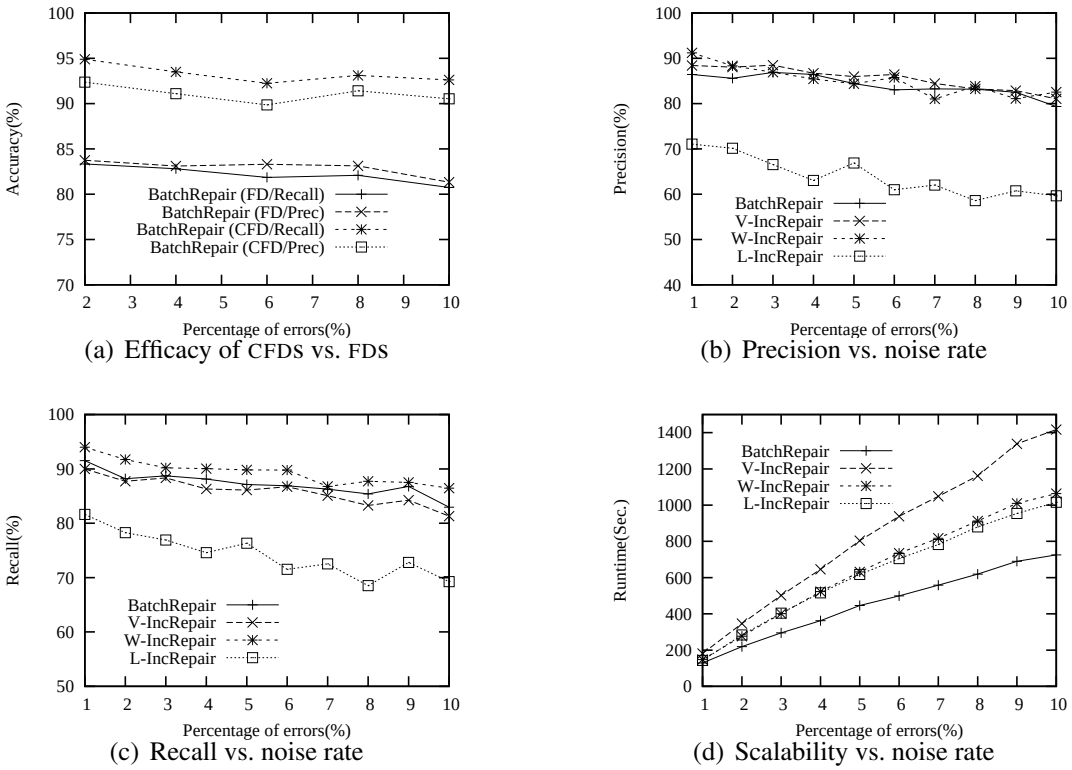
4.4.2 Experimental Results

We now report our findings concerning the accuracy (Precision/Recall) of our algorithms, their scalability in terms of the size of the data, noise rates, and types of violations, and show the efficacy of CFDs vs. FDs in repairing data.

Efficacy of CFDs vs. FDs. We first show that CFDs are indeed more effective than FDs in repairing dirty data. In Fig. 4.7(a), we run BATCHREPAIR on a dataset of 60K tuples and varied the noise rate ρ between 2% to 10%. The upper two curves report the accuracy for our set of CFDs. The lower two curves show the accuracy for the embedded FDs (i.e. the CFDs in which the pattern tableau consists of a single pattern of wildcards only). Figure 4.7(a) shows that patterns improved significantly the accuracy of the repair.

Quality of the repair. We evaluated the data quality of our repairing algorithms. We show the accuracy in terms of *Precision* (Fig. 4.7(b)) and *Recall* (Fig. 4.7(c)) of all our algorithms, i.e. BATCHREPAIR, L-INCREPAIR, V-INCREPAIR and W-INCREPAIR. In these experiments, we varied the noise rate ρ from 1% to 10%. The total database size was fixed at 60K tuples.

Our experiments show that V-INCREPAIR and W-INCREPAIR consistently outperform L-INCREPAIR, while W-INCREPAIR performs slightly better than V-INCREPAIR. The accuracy of W-INCREPAIR is influenced by the quality of the weights, i.e. the choice of a and b. The good performance of V-INCREPAIR is consistent with the expectation that a tuple which has less violations is more likely be a correct tuple. Indeed, algorithm V-INCREPAIR first repairs tuples that are more likely to be correct, which will provide more reliable information when cleaning less accurate dirty tuples subsequently. A similar argument holds



(a) Efficacy of CFDs vs. FDs (b) Precision vs. noise rate

(c) Recall vs. noise rate (d) Scalability vs. noise rate

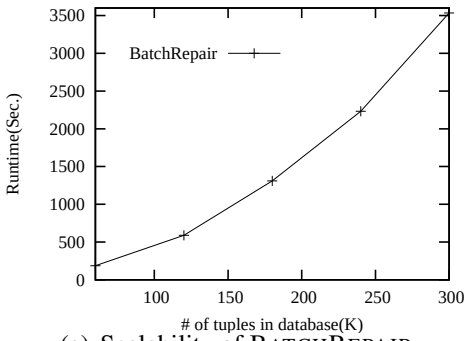
Figure 4.7: Experimental results

for the good accuracy of W-INCREPAIR. Moreover, the running times (Fig. 4.7(d)) of L-INCREPAIR and W-INCREPAIR are similar and slightly better than V-INCREPAIR. Therefore, the improved quality of the latter two algorithms *does not* come at a price, in terms of time.

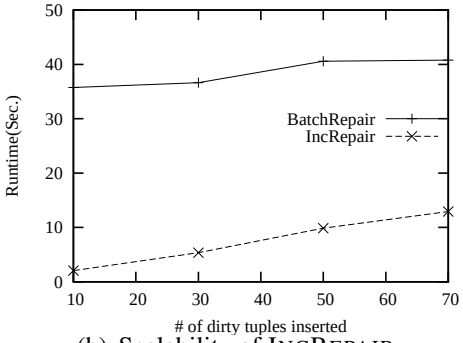
Also in Fig. 4.7(b) and Fig. 4.7(c) we show the accuracy of the repair given by BATCHREPAIR. Although BATCHREPAIR and INCREPAIR are different in nature, the quality of the repairs provided by them is comparable. Note also that the *Precision* and *Recall* decrease slightly with the increase of noise rate, as expected. The values of *Recall* are relatively high, which means that our algorithms can repair most of the errors. *Precision* shows that new noises were introduced when repairing these errors.

In the following, when reporting on the INCREPAIR algorithm we always used V-INCREPAIR, as it consistently gave good results for a wide range of (a,b)-values.

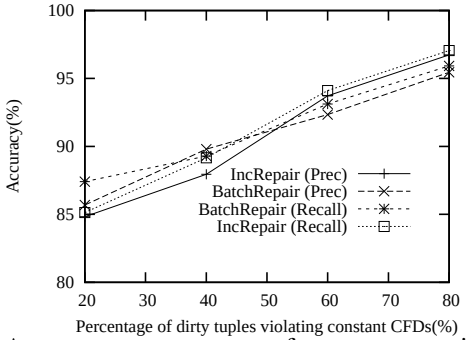
In Fig. 4.8(c) we verify our intuition that CFDs with a constant in their RHS are more informative during the repairing than those with a variable RHS. In this experiment we



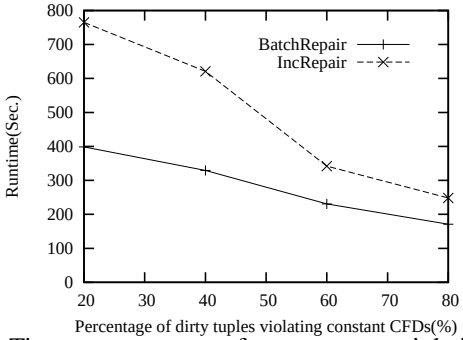
(a) Scalability of BATCHREPAIR



(b) Scalability of INCREPAIR



(c) Accuracy vs. percentage of constant CFD violations



(d) Time vs percentage of constant CFD violations

Figure 4.8: Experimental results

fixed the size of the data to 60K tuples and varied the percentage of violations for constant CFDs *w.r.t.* violations for variable CFDs from 20% to 80%. As can be seen, an increasing number of constant CFD violations enabled both BATCHREPAIR and INCREPAIR to achieve higher accuracy.

Scalability. In the following experiments we investigate the scalability of our algorithms. In Fig. 4.8(a) we show the scalability of BATCHREPAIR. As described in Section 4.2, the overall complexity is governed by the procedure PICKNEXT. Our experience shows that without any further optimization, BATCHREPAIR runs very slow. Therefore, we applied some additional optimizations based on the dependency graph of the CFDs, which help PICKNEXT to select the next CFD to repair. As Fig. 4.8(a) shows, the optimized BATCHREPAIR scales very well for database sizes varying from 60K to 300K tuples. The noise rate was fixed at 5%.

The effectiveness of INCREPAIR, when used in the *incremental* setting, is reported in

Fig. 4.8(b). We started from a clean database consisting of 60K tuples and inserted 10 to 70 tuples. It shows that for small updates INCREPAIR significantly outperforms BATCHREPAIR in this incremental setting, with comparable accuracy (see Figs. 4.7(b) and 4.7(c)). Observe that the running time of INCREPAIR increases faster than that of BATCHREPAIR. Therefore, for large sets of updates BATCHREPAIR is preferable.

The scalability of all our algorithms with respect to noise rate is shown in Fig. 4.7(d). We fixed the data size to 60K tuples and varied the noise rate from 1% to 10%. All algorithms require more time when the data has more noise, as expected. An interesting observation is that BATCHREPAIR is less sensitive to the noise rate because it can repair many tuples simultaneously.

In Fig. 4.8(d) we show that the presence of violations for variable CFDs has a negative effect on the time performance of both BATCHREPAIR and INCREPAIR. This is not surprising since such violations involve multiple tuples.

Summary. Our experimental results demonstrate both the effectiveness and efficiency of our repairing algorithms. (1) We find that all of our repairing algorithms, even the worst-performed L-INCREPAIR, improve the quality of the data. (2) All of our algorithms scale well with the database size. (3) Algorithms BATCHREPAIR and V-INCREPAIR provide repairs that have comparable accuracy. (4) Repair quality decreases when the noise rate increases for all of the algorithms. (5) If violations are mainly caused by constant CFDs, then the algorithms run more efficiently and provide more accurate results. (6) While our algorithms correctly fix noises, they may also introduce new noises. This is an issue not yet well studied by previous work.

These results are based on synthesized data due to the difficulties to obtain verifiable real-life dirty data. Currently, we are not aware of any reasonably large real-life data set which provides both the dirty and the clean versions. Manually verifying the repairing result is not feasible due to the lack of domain knowledge and, more importantly, the prohibitive time involved in it. For example, [GT00] showed that it took a team of 10 analysts 6 months to review and correct a moderate survey. Further experimental studies are pending to the availability of real-life dirty data or data cleaning benchmarks.

Chapter 5

From Relation to XML

In the last two chapters, a data cleaning sub-framework for improving data quality has been presented. In the sub-framework, the data is stored and represented in relational model. Relational databases have dominated information systems for decades. The success of relational databases is largely due to their abilities to store and manipulate huge volume of data efficiently. Such abilities are gained from the well-defined relational data model, the standard language for defining and manipulating relational data, and the efficient implementation of the language with sophisticated indexing and optimisation techniques. The efficiency and reliability of relational database systems has been proven to be essential to numerous applications.

However, since the 1990s, the rapid development of the Internet has changed the picture of information systems. In the past decade, XML has become the primary standard for publishing and exchanging data. As a result, relational data has been increasingly consumed in XML format. In response to this, CLINSE supports the management of the cleaned relational data in XML format through the XML integration and XML security sub-frameworks.

XML is an extremely versatile data format that can represent both *structured* and *semi-structured* data. For instance, XML is widely used to represent *structured documents* (books [OAS06], web pages [W3C00], office documents [ISO06b]), transactions between business partners (ebXML [Ot]), software configurations and registries (UDDI [OAS]), metadata (MPEG7 [ISO01], Dublin Core [Ini03], RDF [W3C04a]), and even vector graphs (SVG [W3C03]), formula (MathML [W3C01]), multimedia (SMIL [W3C04b])...XML

makes it possible to represent and exchange all these classes of data in a standard format.

This flexibility of XML makes it popular to serve as a unified format for data in other models. For example, the relational customer data used in the last two chapters could be easily transformed into XML format.

Example 5.1: Recall the instance of customer relation in Fig. 3.1. It can be naïvely converted into an XML document shown in Fig. 5.1. This XML document will be explained later.

```
<?xml version='1.0'?>
<db>
  <customer>
    <name> Mike </name>
    <country> US </country>
    <city> NYC </city>
    <street> Tree Ave. </street>
    <zip> 10012 </zip>
    <country_code> 1 </country_code>
    <area_code> 607 </area_code>
    <phone_number> 1111111 </phone_number>
  </customer>
  <customer>
    ...
  </customer>
  ...
</db>
```

Figure 5.1: Customer data represented in XML

□

The customer data in XML format has the same structure as the one in relational model: it is only different in syntax. However, in general, the transformation of data from relational model to XML format is non-trivial. In fact, there is a host of research dealing with this problem in the past few years. In this chapter, after a brief introduction to XML, the transformation is illustrated by a more complex example using the framework developed in

[BCF+02, CFJK04].

5.1 XML Data Model

Evolved from SGML (Standard Generalized Markup Language [ISO86]), a meta-language for specifying document markup languages dated back to 1960s, XML (eXtensible Markup Language [BPSM98a]) is a standard for sharing data across different information systems, especially over the Web. Similar to SGML, XML represents information by combining data and meta-data in a tree structure using nested start- and end-tags. XML syntax is introduced below through the customer example:

Example 5.2: The major building blocks of an XML document are *element*s. An element consists a start-, end-tag pair and its enclosed contents. The text of the tag is called the *name* of the element. In Figure 5.1, `<customer> ... </customer>` is an element enclosed by start-tag `<customer>` and end-tag `</customer>`. Such start-, end-tag pair can be arbitrarily nested to form a tree structure with a unique element — enclosed by the outermost pair of tags — as the root of the tree, referred to as the *root* element. In Figure 5.1, the element `<name> ... </name>`, is nested inside `<customer> ... </customer>`, which is in turn enclosed by the root element `<db> ... </db>`. Besides elements, other important building blocks of an XML document are *attribute*s and *PCDATA*s (Parsed Character DATA). Unlike elements, neither attributes, nor PCDATAs are allowed to be nested. That is to say, both of them should only appear at the leaf nodes of the tree structure. More specifically, an attribute can be placed inside the start tag of any element as a name value pair separated by the equality sign ("="); a PCDATA item is, by contrast, either placed inside an innermost start-, end-tag pair as a block of texts, or mixed with elements inside arbitrary tag pair. For instance, the text `NYC` enclosed by tag pair `<city> </city>` is a PCDATA item.

The information in an XML document organized as above forms a tree with its nodes representing elements, attributes or PCDATA items and its edges corresponding to the containment between them. The XML tree for the customer data is shown in Figure 5.2. In an XML tree, each inner node is *labelled* with the name of an element or an attribute; each leaf node shows the name of an element, the value of a PCDATA item or an attribute. A node corresponding to a PCDATA item is referred to as a *text* node. Figure 5.2 shows text nodes

in italic font. For all the non-attribute children of a node, there is a *document order* defined between them. The document order is the order in which the first character of each node occurs in the XML document: the root node will be the first node; element nodes occur before their children; the attribute nodes of an element occur before the children of the element; the relative order of attribute nodes is not defined. In Figure 5.2, the document order is `db, customer, name, Mike, country, ..., phone_number, 1111111, customer, ...`

Elements, attributes and PCDATAs are most widely used information items in an XML document. In fact, a real-world XML document can contain up to eleven different types of information items as specified in XML Information Set [CT04]. A node in an XML tree can be element, attribute, text, document, comment, processing instruction, or namespace [FMM+07]. For convenience of presentation, following most work in the literature, this thesis considers a simplified XML model which consists elements and PCDATAs (i.e., text nodes), and thus a document order is always defined between two nodes in an XML tree.

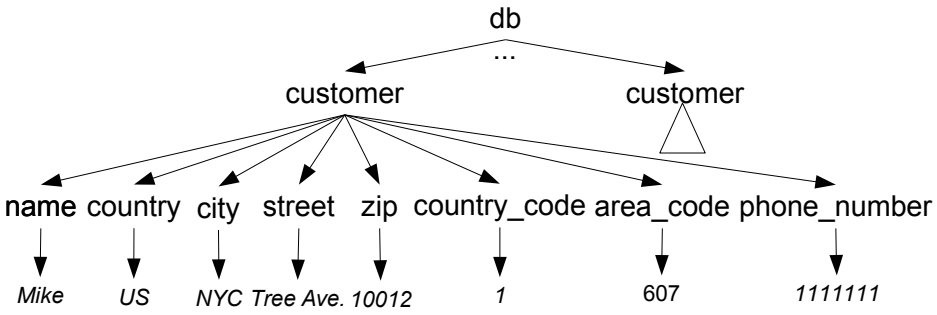


Figure 5.2: XML tree for the customer data

□

Following the models used in [KSS03, Nev02a, Lib06], in this thesis, an XML document is modelled as a *node-labelled, ordered, unranked* tree. An *unranked* tree is a tree in which there are no restrictions on the number of children a node can have. A tree is *ordered* if there exists an order defined among the nodes in the tree. For an XML tree, this order is the document order described earlier. The nodes in an XML tree are *labelled* using the element name with the exception of text nodes being leaves, which are assigned values from an infinite domain. Such a tree captures both the element structure of an XML document and its data values.

We shall use $\mathcal{T}$ to denote a set of trees. For a tree $t \in \mathcal{T}$, each node of t is defined by a

string of numbers: the root of t is ε; the i-th children of a node n is $n \cdot i$ which denotes the concatenation of string n and number i. The set of nodes of a tree t forms the *domain* of t, denoted by D. Two binary relations are defined on this tree domain: a *child* relation $R_{\downarrow}$ and a *next-sibling* relation $R_{\rightarrow}$. For two nodes $n_1, n_2 \in D$

$$\begin{aligned} R_{\downarrow}(n_1,n_2) &\iff n_2 = n_1 \cdot i \text{ for some } i \in \mathbb{N} \\ R_{\rightarrow}(n_1,n_2) &\iff n_1 = n_0 \cdot i \text{ and } n_2 = n_0 \cdot (i+1) \text{ for some } n_0 \in \mathbb{N}^* \text{ and } i \in \mathbb{N} \end{aligned}$$

The tree domain D is partitioned into two disjoint sets: element nodes D_e and text nodes D_t. D_e and D_t satisfies $D = D_e \cup D_t$ and $D_e \cap D_t = \emptyset$. As mentioned before, text nodes D_t consist only the leaf nodes of an XML tree. However the opposite is not true: a leaf node can also be an empty element in the form of `<a/>`.

Let Σ be a finite alphabet of labels (element names) and $|\Sigma| = k$. We define k unary relation $P_l, l \in \Sigma$ on tree domain D_e

$$P_l(n_1) \iff \text{node } n_1 \in D_e \text{ is labeled with } l \in \Sigma$$

Let V be an infinite alphabet of values (data value of a text node). We define two functions: a *labeling* function $\lambda : D_e \rightarrow \Sigma$, and a *value* function $\nu : D_t \rightarrow V$. For an element node $n_1 \in D_e$ and a text node $n_2 \in D_t$

$$\begin{aligned} \lambda(n_1) = l &\iff P_l(n_1), l \in \Sigma \\ \nu(n_2) = v &\iff \text{the value of the text node } n_2 \text{ is } v \in V \end{aligned}$$

Now an XML tree is defined as

$$\mathcal{T}_{\Sigma,V,\rightarrow} = (D, \Sigma, V, R_{\downarrow}, R_{\rightarrow}, \lambda, \nu)$$

Alternatively, we can define it as

$$\mathcal{T}_{\Sigma,V,\rightarrow} = (D, \Sigma, V, R_{\downarrow}, R_{\rightarrow}, (P_l)\, l \in \Sigma, \nu)$$

by replacing the labelling function λ with a set of predicates $(P_l)\ l \in \Sigma$.

If we ignore the values in an XML document, i.e., we only keep element nodes in an XML tree, we will get a navigational part of the document. The corresponding XML trees are often referred to as Σ-trees, denoted by $\mathcal{T}_{\Sigma,\rightarrow}$

$$\mathcal{T}_{\Sigma,\rightarrow} = (D, \Sigma, R_{\downarrow}, R_{\rightarrow}, (P_l)\, l \in \Sigma)$$

A labelled, unordered tree is defined as

$$\mathcal{T}_\Sigma = (D, \Sigma, R_\downarrow, (P_l)\ l \in \Sigma)$$

In this thesis, an XML document is modelled as $\mathcal{T}_{\Sigma,V,\rightarrow}$.

There are two levels of correctness of an XML document: well-formed document and valid document. If an XML document adheres to the syntax rules of the XML specification, we say it is *well-formed*. If, in addition, it satisfies the constraints specified in a *schema*, we say it is *valid* against the schema. Although an XML document must be well-formed, it is not always required to be valid. Usually a well-formed document without a schema is suitable for document oriented applications due to its flexibility; while a valid document is often required for database oriented applications because the schema is essential for formulating queries and storing data efficiently. The processing of a valid XML document, as that of a relational database, needs both data definition languages and data manipulation languages. But unlike relational databases, in which the data definition and manipulation are both achieved by SQL standard, XML has independent data definition and manipulation languages which are separated from each other.

5.2 XML Data Definition

Although a number of schema languages, which are in analogy to the data definition languages of databases, have been proposed for XML, only four of them are standardized: Document Type Definitions (DTDs [BPSM98b]) and XML Schema (XSD [TBMM01]) are W3C recommendations; RELAX NG ([CM01]) and Schematron ([ISO06a]) are parts of ISO/IEC 19757 Document Schema Definition Languages (DSDL) standard. XML DTDs are simplified from SGML DTDs. XML Schema is evolved from earlier proposals such as DCD, DDML, SOX, and XDR. RELAX NG is based on Murata Makoto's RELAX and James Clark's TREX. Schematron is influenced by XPath.

Two approaches have been used to define the structure of a document: one is to define the document structures by derivation trees of grammars; the other is to define the structures by using a set of rules to assert the presence or absence of patterns in trees. Accordingly, these schema languages can be classified into two categories: *grammar-based* and *rule-*

based. DTDs, XML Schema and RELAX NG are grammar-based. Schematron is rule-based.

Example 5.3: To demonstrate the schema languages, DTDs for the customer XML document are shown in Figure 5.1.

Customer DTD D:

```
<!ELEMENT db       (customer*)>
<!ELEMENT customer (name, country, city, street, zip,
                   country_code, area_code, phone_number )>
<!ELEMENT name     (#PCDATA)
/* Other #PCDATAs are omitted here.  */
```

Figure 5.3: DTDs for the customer XML document

□

There are close connections between grammar-based schema languages and formal languages. DTDs describe an XML document as a derivation tree of extended context-free grammars (ECFG), which are context-free grammars (CFG) with regular expressions as right-hand sides ([Nev99]). Although ECFGs generate the same class of string languages as CFGs, their derivation trees are different. As a consequence, the structures of the XML documents they defined are also different.

Without loss of generality, we normalize the ECFG productions and define a DTD as (Ele, P, r), where Ele is a finite set of *element types* which equals to $\Sigma \cup \{str, \varepsilon\}$, str is a type for text node, ε is a type for empty word; r is a distinguished type in Ele, called the *root type*; P defines the element types: for each A in Ele, $P(A)$ is a regular expression of the following form:

$$\alpha ::= \mathsf{str} \mid \varepsilon \mid B_1, \ldots, B_n \mid B_1 + \ldots + B_n \mid B^*$$

where B is a type in Ele (referred to as a *child type* of A), and '$+$', ',' and '$*$' denote disjunction, concatenation and the Kleene star, respectively (we use '$+$' instead of '$|$' to avoid confusion). We refer to $A \rightarrow P(A)$ as the *production* of A. It has been shown in [BCF$^+$02] that all DTDs can be converted to this form in linear time by introducing new

element types. To simplify the discussion we do not consider XML attributes, which can be easily incorporated.

Example 5.4: In the DTDs for the customer XML document shown in Figure 5.3, the set of element types Ele is {`db, customer, name, ...`}. Among them, `db` is the root element r. The element type `db` is defined by the production `db` $\rightarrow$ `customer`. The element `customer` is in turn defined by the production `customer` $\rightarrow$ `name, country, ...`, and the element `name` is defined by `name` $\rightarrow$ `str`. Other element types are defined in the same way. More complex DTDs can be found in Figure 5.6. □

An XML document (tree) T *conforms to* a DTD D if (1) there is a unique node, the *root*, in T labeled with r; (2) each node in T is labelled either with an Ele type A, called an A *element*, or with PCDATA, called a *text node*; (3) each A element has a list of elements and text nodes as its children such that their labels are in the regular language defined by $P(A)$; and, (4) each text node carries a string value (PCDATA) and is a leaf of the tree. We call T a *document* (instance) of D if T conforms to D.

Customer DTD D':

```
<!ELEMENT db       (customer*)>
<!ELEMENT customer (name, country, city, street, zip, phone)>
<!ELEMENT country  (name, code)
<!ELEMENT city     (name, code)
<!ELEMENT name     (first_name, last_name)
<!ELEMENT name     (#PCDATA)
/* Other #PCDATAs are omitted here.  */
```

Figure 5.4: Illegal DTDs for the redesigned customer document

In an XML document defined by DTDs, an element type depends only on the name of the element: it is independent of the context of the element in the document. This is why we can use the element name to identify the element types in our DTD definition. But this context independence imposes restrictions on the types being defined. For example, if the DTDs for the customer data are designed to group country name and country code together under a `country` element and rename them to `name` and `code` element respectively, as shown in Figure 5.4, the DTDs would be illegal due to the fact that there are two types, and

consequently two definitions, for the `name` element, that causes conflicts and is not allowed in DTDs. In fact, it is unable to define such a schema using DTDs because the element type of `name` element is not solely determined by the element name, but also dependent on its context: it has sub-element `first_name` and `last_name` if it is below the `customer` element; otherwise it has only PCDATA content. To define such schemas, XSD or RELAX NG is needed. The XSD definition is shown in Figure 5.5. Note that although there are two definitions for `name` element type, they are distinguishable because the definitions are embedded into different parent types, i.e. `customer` and `country`.

```
<xs:element name="db">
  <xs:complexType> <xs:sequence>
    <xs:element name="customer" maxOccurs="unbounded">
      <xs:complexType> <xs:sequence>
        <xs:element name="name"/>
          <xs:complexType> <xs:sequence>
            <xs:element name="first_name" type="xs:string"/>
            <xs:element name="last_name" type="xs:string"/>
          </xs:sequence> </xs:complexType>
        </xs:element>
        <xs:element name="country">
          <xs:complexType> <xs:sequence>
            <xs:element name="name" type="xs:string"/>
            <xs:element name="code" type="xs:string"/>
          </xs:sequence> </xs:complexType>
        </xs:element>
        ...
        <xs:element name="phone" type="xs:string"/>
      </xs:sequence> </xs:complexType>
    </xs:element>
   </xs:sequence> </xs:complexType>
</xs:element>
```

Figure 5.5: XML Schema for the redesigned customer document

Therefore, Grammar-based schema languages can be further divided into *context insensitive* ones and *context sensitive* ones depending on if element types are solely determined by element names. DTDs are context insensitive schema language. XML Schema and RELAX NG are context sensitive languages. RELAX NG is the most impressive one among the three. It corresponds to robust and well-understood unranked regular tree languages [MNSB06, BKMW01]. Although context independence poses limitations on expressiveness, it has a good effect: the type of an element can be decided without referencing the schema definition. This is consistent with the self-description feature of XML and makes XML documents easier to understand. In this thesis, XML documents are always defined by the normalized DTDs.

5.3 XML Data Manipulation

Like XML data definition languages, there are several standard manipulation languages for XML data. These languages aim at different purposes.

XQuery. In relational databases, SQL is used to retrieve and modify data in databases; for XML data, the first task is achieved by XQuery [Cha07] and the language for the second task is still under development [CFR06].

XSLT. Relational databases are designed and optimized for data centric tasks. In contrast, XML is developed for both data centric and document centric tasks. In document centric applications, the task of transforming documents between different representations is often required. Consequently, another type of data manipulation languages designed for data transformation is desired for these applications. The standard transformation language for XML is XSLT [Cla99].

XPath. Since XML data is modeled as trees, any XML manipulation language needs to navigate trees. This functionality is separated out from XQuery and XSLT as an independent language called XPath [CD99]. There are two versions XPath: XPath 1.0 [CD99] and XPath 2.0 [Ber07].

These languages for XML data manipulation are often generally referred to as *XML query languages*. A bulk of work has been published for the evaluation and optimisation of XML query languages in the last decade. Many theory aspects of XML query languages

have been investigated, too. Although most of the work is concerned with XPath, in fact, it often deals with a fragment of XPath or an extension of a fragment of XPath.

A small fragment of XPath, referred to as $\mathcal{X}_{\cup}^{\downarrow}$, is defined as follows:

$$\begin{aligned} p &::= /p \mid p/p \mid p \cup p \mid x :: t, \\ x &::= \varepsilon \mid \downarrow \\ t &::= l \end{aligned}$$

where p is the XPath expression and the start production, x stands for axis relations and t denotes node tests, $\cup$, ε, $\downarrow$ and l denote union (i.e. "|" in W3C syntax), self axis, child axis and an element name (label) in Σ. Note the child axis $\downarrow$ is a simplified notation of the child relation $R_{\downarrow}$ defined in the data model. In this fragment, the only node test allowed is to match a label of an element between an XPath expression and an XML tree, and the axis relations are restricted to self and child axes. This is a basic path fragment without filters and recursions. It is the smallest fragment studied in [BFK05] which shows that this fragment is closed under intersection and union.

A larger fragment is defined by allowing filters, boolean connectives in filters, wildcards in node tests, and all downward axes defined by W3C:

$$\begin{aligned} p &::= /p \mid p/p \mid p \cup p \mid x :: t[q] \cdots [q], \\ q &::= q \wedge q \mid q \vee q \mid \neg q \mid p \mid p/text() = c, \\ x &::= \varepsilon \mid \downarrow \mid \downarrow^*, \\ t &::= l \mid * \end{aligned}$$

where $*$ in node tests denotes wildcard, $\downarrow^*$ denotes the recursive *descendant-or-self* axis (i.e. "//" in W3C syntax), the expressions enclosed in $[\cdot]$ are *filters*, also called qualifiers or predicates in literature, $\wedge, \vee, \neg$ and c inside the filter denote conjunction, disjunction, negation and a string constant, respectively. Note $*$ has two meanings: it denotes wildcard in node tests and Kleene star elsewhere. The features of a fragment could be summarized as $\mathcal{X}_{p;[q]}^{x;t}$, where p, q, x, t represent the features allowed in path expressions, filters, axis relations and node tests, respectively. Thus, this fragment can be represented as $\mathcal{X}_{\cup;[\neg,=]}^{\downarrow,*;*}$ (here $*$ before the semicolon means allowing recursive axes, $*$ after the semicolon denotes wildcard in node tests, $\wedge$ and $\vee$ are not included in the summary because they can be

expressed using filters and $\cup$). This fragment includes most features in downward XPath and is used by [FCG04, FYL$^+$05] in XML security and XML to SQL query translation. The proper subsets of this downward fragment, $\mathcal{X}^{\downarrow,*;*}$, $\mathcal{X}^{\downarrow,*}_{;[]}$, $\mathcal{X}^{\downarrow,*}_{;[]}$ and $\mathcal{X}^{\downarrow,*;*}_{;[]}$ are used in [MS04] to study the containment and equivalence problems. Other fragments larger than $\mathcal{X}^{\downarrow}_{\cup}$, such as $\mathcal{X}^{\downarrow,\uparrow,*}_{\cup;[]}$ and its variants, are studied in [BFK05].

[GKP02, GKP05a] propose a fragment, called *Core XPath*, which can be seen as the logical core of XPath 1.0. It is obtained by introducing more axes and removing the equality in filters:

$$
\begin{aligned}
p &::= /p \mid p/p \mid p \cup p \mid x :: t[q] \cdots [q],\\
q &::= q \wedge q \mid q \vee q \mid \neg q \mid p,\\
x &::= \varepsilon \mid \downarrow \mid \uparrow \mid \downarrow^+ \mid \uparrow^+ \mid \downarrow^* \mid \uparrow^* \mid \rightarrow^+ \mid \leftarrow^+ \mid (\uparrow^* / \rightarrow^+ / \downarrow^*) \mid (\uparrow^* / \leftarrow^+ / \rightarrow^*),\\
t &::= l \mid *
\end{aligned}
$$

where $\uparrow, \downarrow^+, \uparrow^+, \uparrow^*, \rightarrow^+, \leftarrow^+, (\uparrow^* / \rightarrow^+ / \downarrow^*), (\uparrow^* / \leftarrow^+ / \rightarrow^*)$ denote *parent, descendant, ancestor, ancestor-or-self, following-sibling, preceding-sibling, following and preceding* axes, respectively. Here, $\rightarrow$ is a simplified notation of the next-sibling relation $R_{\rightarrow}$ defined in the data model. $\uparrow$ and $\leftarrow$ are the inverse of $R_{\downarrow}$ and $R_{\rightarrow}$, respectively. In fact, all axes defined by W3C, except for the attribute and namespace axis relations, are included in this fragment. This fragment can be summarized as $\mathcal{X}^{\downarrow,\uparrow,\rightarrow,\leftarrow,*;*}_{\cup;[\neg]}$. When it is extended to also include non-transitive sibling axes $\rightarrow$ (*next-sibling* axis) and $\leftarrow$ (*previous-sibling* axis), the new fragment is also called *navigational XPath* because it includes all the navigational features of XPath, while excludes the manipulation of data values such arithmetics and string manipulations. Core XPath queries can be evaluated in time $O(|D| \cdot |Q|)$, that is, time linear in the size of the query and of the data tree [GKP05a]. Arbitrary XPath queries can be evaluated in time $O(|D|^4 \cdot |Q|^2)$ and space $O(|D|^2 \cdot |Q|^2)$ where $|D|$ is the size of the XML document and $|Q|$ is the size of the XPath query [GKP05b].

Recently, [CM07] proposes *Core XPath 2.0*, which includes variables, more set opera-

tions on paths, node comparison in filters and for constructs:

$$
\begin{aligned}
p &::= /p \mid p/p \mid p \cup p \mid p \cap p \mid p \setminus p \mid x :: t[q] \cdots [q] \mid r \mid for\ \$i\ in\ p\ return\ p,\\
q &::= q \wedge q \mid q \vee q \mid \neg q \mid p \mid r\ is\ r,\\
x &::= \varepsilon \mid \downarrow \mid \uparrow \mid \downarrow^{+} \mid \uparrow^{+} \mid \downarrow^{*} \mid \uparrow^{*} \mid \rightarrow^{+} \mid \leftarrow^{+},\\
t &::= l \mid *\\
r &::= \cdot \mid \$i
\end{aligned}
$$

where r is node reference, $\cap$ and $\setminus$ denote intersect and except operators, respectively, *is* denotes the node comparison operator in filters, $\cdot$ is short for $\varepsilon :: *$ and $\$i$ is a variable. This fragment is summarized as $\mathcal{X}^{\downarrow,\uparrow,\rightarrow,\leftarrow,*;*}_{\cup,\cap,\setminus,\$,for;[\neg,is]}$. It can be seen as the logical core of XPath 2.0. Most features in XPath 2.0, such as the constructs of *if-then-else*, *some/every-in-satisfies* can be expressed in this fragment.

An important extension of XPath is *regular* XPath which is proposed and studied in [Mar04b]. The downward regular XPath is defined as follows:

$$
\begin{aligned}
p &::= /p \mid p/p \mid p \cup p \mid x :: t[q] \cdots [q] \mid p^{*},\\
q &::= q \wedge q \mid q \vee q \mid \neg q \mid p \mid p/text() = c,\\
x &::= \varepsilon \mid \downarrow\\
t &::= l \mid *
\end{aligned}
$$

where the $*$ outside of the node tests denotes Kleene star. Regular XPath [Mar04b] extends regular expressions by allowing filters, and extends XPath by supporting Kleene closure p^{*} as opposed to the restricted recursion $\downarrow^{*}$ (i.e., '//', the *descendant-or-self axis*). This extension is summarized as $\mathcal{X}^{\downarrow;*}_{\cup,*;[\neg,=]}$. Note that $\downarrow^{*}$ (i.e., '//') in downward XPath $\mathcal{X}^{\downarrow,*;*}_{\cup;[\neg,=]}$ is expressible in downward regular XPath $\mathcal{X}^{\downarrow;*}_{\cup,*;[\neg,=]}$ as $(\downarrow :: *)^{*}$, where the $*$ inside of $(\cdot)$ denotes the wildcard in node tests and the $*$ outside of $(\cdot)$ denotes Kleene star.

Other extensions, such as Conditional XPath, Caterpillar Expression, Looping Caterpillar, are defined in [Mar04b, Mar04a, GM05]. More background on XPath can be found in a recent survey [BK06].

In this thesis, the downward fragments of XPath and regular XPath, i.e., $\mathcal{X}^{\downarrow,*;*}_{\cup;[\neg,=]}$ and $\mathcal{X}^{\downarrow;*}_{\cup,*;[\neg,=]}$ are used to study the XML security problem (see Chapter 7).

Both XQuery and XSLT 2.0 contain more features than XPath 2.0 and are turing-complete [Kep04]. XQuery extends XPath 2.0 by adding features such as FLWR expressions (for-let-where-return), element constructors, function definitions (including recursive functions), static typing, etc. In this thesis, XQuery is used in XML data integration (see Chapter 6).

5.4 XML Views

The notion of views is essential in databases [AHV95, RG00]. The motivation behind the view mechanism is to tailor how users see the data. It allows various users to see the data from different viewpoints. The need for such a concept is first witnessed in traditional databases. In XML data management, views are required for the same reason: different users sharing XML data may have different needs and may want to see the same data differently. Furthermore, since XML data is widely used as a common model for heterogeneous data, the use of views is even more essential than in traditional databases. A lot of work on XML views [Abi99, FCG04, SKS$^+$01a, AMN$^+$01a, BGK$^+$02, DESR03, BCF04] has been published since the early years of XML research.

In relational databases, a *view* is a virtual or logical table composed of the result set of a pre-compiled query. A view specification for XML data will primarily rely, like for relational views, on a data model and a query language. But unlike relational views, both the data model and the query language are more diverse.

Based on the model of the underlying data sources, XML views can be classified as XML views over XML data (V_X^X), XML views over non-XML data, say, relational data (V_R^X), and XML views over heterogeneous data (V_H^X).

All these categories have been found useful in a variety of fields: V_R^X views have been intensively investigated in *XML publishing* [FKS$^+$02, SSB$^+$01b, BCF$^+$02, LBKN03] and in *XML storage* [DFS99, BP05]; V_X^X views are critical in *XML security* [FCG04], *XML integration* [PA05] and *XML data exchange* [AL05]; V_H^X views are essential to *XML integration* [FGXJ04, YP04, DT01]. These categories disclose the relationships between different applications of the XML views. In this thesis, XML publishing is discussed in Section 5.5; XML integration and security are presented in Chapter 6 and 7.

As pre-compiled queries, XML views may be *materialised* (i.e., a physical copy of the

view is stored and maintained) or *virtual* (i.e., relevant information about the view is computed as needed). The former case is preferred in data exchange or read-only applications such as data warehousing, especially when large part of the data included in the view is needed each time. However, in other applications, it introduces the overhead of materialisation and the difficulty of view maintenance. These problems are more evident when multiple views of a large document are materialised at the same time. For virtual views, queries against the view have to be unfolded to incorporate the view definition and translated to queries against the underlying XML documents (V_X^X) or underlying tables (V_R^X). This is generally referred to as *query rewriting* or *query composition*. For V_R^X, it is also referred to as *XML-to-SQL query translation*.

Depending on whether the XML view is virtual or materialised, there are different problems associated with XML views. *View definition*, *query evaluation and optimisation* are fundamental problems in both. However, for materialised views, the problems of *view materialisation*, *view maintenance* are raised. In contrast, for virtual views, the problem of *query rewriting* is important.

As in traditional databases, the users should not worry about the difference between XML views and underlying XML documents when querying the data. At a first glance, any language suitable for querying XML documents should be suitable for querying XML views. However, this is not true because the queries posed over the views need to be rewritten into the queries over underlying XML documents and thus they should be closed under rewriting, as we will explain in Chapter 7.

One of the challenges in querying XML views arises from recursively defined XML views. We say an XML view is *recursive* when the DTD (Document Type Definition) for the view is recursive, i.e. the graph derived from the DTD is cyclic. In addition to the recursion in the DTD, the query posed over an XML view could also be recursive, such as the descendant axis ("//") in XPath. Both of the two types of recursion are ubiquitous. Choi[Cho02] showed, out of the 60 DTDs analysed, more than half (35) of them are recursive. Recursive queries appear in any path expressions that uses the descendant ("//"), ancestor, following or preceding axis.

This thesis will focus on both materialized and virtual V_X^X views in the context of XML integration and security, respectively. So query rewriting, evaluation, optimisation and view materialization are the major technical issues to be tackled. In the next section, we

will discuss how relational data is transformed to XML format in CLINSE.

5.5 XML Publishing

Despite the excitement surrounding XML, most business data, even in new web-based applications, continues to be stored in relational database systems. Relational database uses proprietary schema which is not suitable for direct data exchange; while XML uses public schema (e.g. DTD, XML Schema) which allows the data in XML format to be exchanged regardless of the platform on which it is stored or the data model in which it is represented. A common way to exchange data currently residing in relational databases is to first convert the data to XML documents, then integrate it with the XML data from other sources, and finally send the integrated XML data over the network to another party. The transformation from relation to XML is referred to as *XML publishing*. The published XML document could be regarded as a *view* of the underlying relational data.

There have been substantial interests in finding ways to efficiently publish existing (object-)relational data to XML format. XPERANTO [SKS+01a, SSB+01a, CFI+00], SilkRoute [FKS+02] and MARS [DT03] use similar view definition mechanisms: they first convert the relational data to a low level "canonical" XML view (it is called "default" XML view in XPERANTO) and then use XQuery to define the final view on top of the "canonical" view. Whereas SilkRoute uses declarative *view forests* as the intermediate representation, XPERANTO uses the more procedural *XML Query Graph Model* (XQGM). ROLEX [BGK+02, LBKN03] and XSLT2SQL [JMS02] adopt the internal representation (view forests) of SilkRoute to *schema-tree query* and *view tree*, respectively, and expose them to end users as view definition languages.

In practice, XML publishing is often done with a predefined "schema". A community agrees on a certain schema, and subsequently all members of the community exchange their data *w.r.t.* the predefined schema, by ensuring their published (*target*) XML data to conform to the fixed schema. This is called *schema-directed XML publishing*. More specifically, it can be stated as follows: given a DTD D, to define a view σ for relational databases I such that $\sigma(I)$ is an XML document conforming to D. The need for schema conformance is particularly evident in cases where the published XML data needs to be integrated: it is hard to specify the integration to combine the published data with unknown or frequently

changed schemas. However, it is nontrivial to ensure schema conformance in XML context. The difficulty is introduced by, among others, recursion in a target schema.

In response to this, [BCF$^+$02, CFJK04] proposes an approach for schema-directed publishing of relational data into XML format, based on the novel notion of *attribute transformation grammars* (ATGs). ATGs provide guidance on how to define views conforming to *target* schemas (DTDs) and better still, they automatically ensure schema conformance. A middleware system [CFJK04] that supports both schema-directed XML publishing based on ATGs, and incremental updates of XML views created by ATGs is provided in CLINSE.

Given an arbitrary target DTD D, an ATG defines a view as follows: (1) For each element type A in D, it defines a variable $\$A$; intuitively, each A element in an XML tree is to have a variable $\$A$, which contains a single relational tuple as its value. (2) For each element type definition (production) $A \rightarrow \alpha$ in D, where α is a regular expression, it specifies a set of semantic rules such that for each element type B in α, there is a rule for computing the values of $\$B$ via an SQL query; the query is treated as a function that may take $\$A$ as a parameter. Given a relational database I, the ATG is evaluated top-down: start at the root element type of D, evaluate semantic rules associated with each element type encountered, and create nodes following the DTD to construct the target XML tree. The values of the variable $\$A$ are used to control the construction.

As an example, consider again publishing the relational customer data introduced in Chapter 3 into XML data. To show the advanced features of XML publishing, now suppose that the organization which maintains the customer data is a hospital, i.e., the customers are patients. In addition to the data recorded in the customer relation, we maintain more information by another three relations: family records the RELATIONSHIP (e.g., parent) between a patient/person (identified by ID1) and one of his family members (identified by ID2); person and history maintain medical history of a family member by his ID, BLOODTYPE and all the DISEASE s he has ever been diagnosed of. The customer relation in the last two chapters is also augmented to record the ID of a patient and is renamed as patient relation (keys are underlined).

Now one wants to construct a target XML document T that contains all the patents from Edinburgh (`EDI`) along with their family medical history. Furthermore, T is required to conform to the DTD D_0 given in Fig. 5.6. Observe that D_0 is *recursive:* a `person` may have other `person`s as its `family` member; this leads to XML trees of unbounded depths.

Source relational schema R_0:

```
patient(ID, NAME, CITY, STR, ZIP,...)
family(ID1, ID2, RELATIONSHIP)
person(ID, BLOODTYPE)
history(ID, DISEASE)
```

Target DTD D_0:

```
<!ELEMENT hospital (patient*)>
<!ELEMENT patient  (name, address, family)>
<!ELEMENT address  (street, city, zip)>
<!ELEMENT family   (person*)>
<!ELEMENT person   (relationship, bloodtype, diseases, family)>
<!ELEMENT diseases (disease*)>
/* #PCDATA is omitted here.  */
```

Figure 5.6: Example of a source schema and a target DTD

An ATG σ_0 specifying the publishing is shown in Fig. 5.7. When being evaluated over the hospital database, σ_0 produces a target XML tree T , as follows.

(1) It first creates the root element, `hospital`, and then triggers the rules associated with the production `hospital` $\rightarrow$ `patient*`. Observe that the production contains a Kleene star; thus there is no bound on the number of the `patient` children of the root. These children are determined by the evaluation of the SQL query Q_1 over the hospital database, which returns all the tuples for the `patient`s living in Edinburgh. For each t of these tuples, a `patient` element is created as a child of the root, carrying t as the value of its variable $\$patient$. The operator "$\leftarrow$" in the rule denotes the iteration for generating the `patient` children, corresponding to the Kleene star.

(2) At each `patient` element p_a, the XML tree T is expanded by generating the children of p_a. In contrast to the last case, the production for `patient` tells us that p_a has exactly three children: `name`, `address` and `family`. The variables associated with these children are assigned values extracted from fields of the parent variable $\$patient$, e.g. $\$family$ inherits

hospital → **patient***

Q_1: $patient ← **select** id, name, str, city, zip **from** patient

patient → **name**, **address**, **family**

$name = $patient.name, $address = $patient

$family = $patient.id

address → **street**, **city**, **zip**

$street = $address.str, $city = $address.city

$zip = $address.zip

family → **person***

Q_2: $person ← **select** p.id, p.relationship, p.bloodtype
from person p, family f
where f.id1 = $family.id **and** f.id2 = p.id

person → **relationship**, **bloodtype**, **diseases**, **family**

$relationship = $person.relationship, $bloodtype = $person.bloodtype,

$family = $person.id $diseases = $person.id

diseases → **disease***

Q_3: $disease ← **select** h.disease
from history h
where h.id = $disease.id

Figure 5.7: An example ATG σ_0

the value $\$patient.id$.

(3a) Subsequently, the `address` element a is expanded in the same way. Three children, `street`, `city` and `zip` of a are created by inheriting values from fields of the variable $\$address$.

(3b) At each `family` element f, the target tree T is further expanded as follows. The SQL query Q_2 finds the ids of all the persons related to the current patient (person) p_a (p_e) in the `family` relation, by using $\$family.id$ as a constant parameter; it then extracts tuples

from the `person` relation using these *id*s. For each t' of these tuples, a `person` child of f is created carrying t' as the value of its variable.

(4) At each `person` element p_e, the XML tree T is again expanded in a similar way as described in (2). Exactly four children of p_e: `relationship`, `bloodtype`, `diseases` and `family` are generated with variables inheriting values from fields of the parent variable $\$person$.

(5a) Similarly, at each `diseases` child ds of `person` element p_e, the SQL query Q_3 extracts all the `disease` tuples related to person p_e from the `history` relation, by using $\$diseases.id$ as a constant. For each of these tuples a `disease` child of ds is generated.

(5b) The `family` child of `person` element p_e is in turn processed as described in (3b).

Steps (3b) – (5b) are repeated until the target tree T cannot be further expanded, i.e. when all the `person`s at the leaves of T are no longer composed of other `person`s as his family members. At this point the evaluation of the ATG is completed.

ATG has several salient features. First, when the evaluation of an ATG terminates, the target XML tree generated is guaranteed to conform to its embedded DTD. Second, it adopts a *data-driven* semantics: the expansion of an XML tree in the recursive case is determined by the source data. Third, it is easy to use ATGs to specify schema-directed XML publishing. The DTD productions provide a guidance on how to write semantic rules to expand the tree that conforms to the DTD. There is no need to learn a new language: one can write ATGs as long as she/he knows SQL and DTD. In [BCF+02], sophisticated evaluation and optimization techniques have been developed for ATGs.

5.6 Summary

In this chapter, using the formalism developed in [BCF+02, CFJK04], a method to transform the cleaned relational data to XML data is described. The background of XML data management, including the data model, schema languages, query languages, and XML views is provided. In the next two chapters, the sub-frameworks in CLINSE to integrate and secure data will be presented.

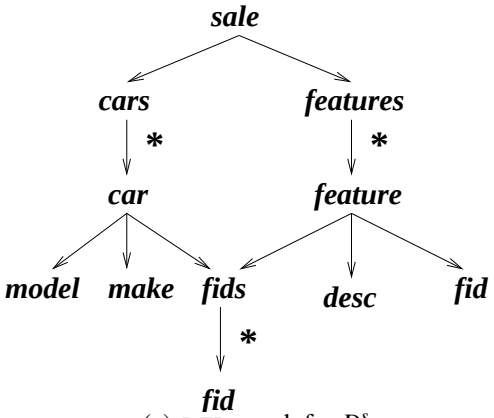
Chapter 6

Schema Directed Integration of the Cleaned Data

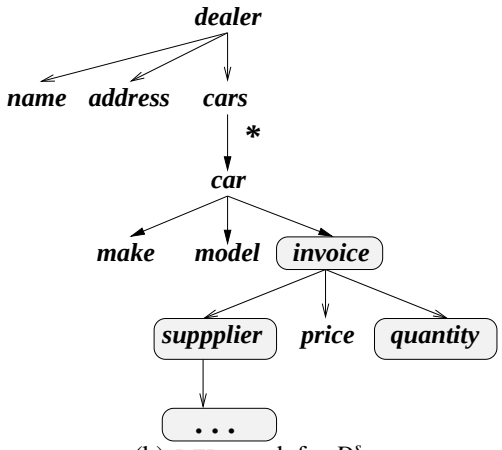
XML [BPSM98a] is rapidly emerging as the dominant standard for data representation and exchange on the Web. The ubiquity of XML, in conjunction with the diversity of next-generation Web applications that rely on it as a data-exchange format, clearly highlights the need for effective XML integration tools, i.e. tools that can efficiently collect data from multiple distributed XML sources and incorporate them in a target XML document. In practice, such XML integration is typically DTD-*directed* – that is, the integration task is constrained by a predefined DTD that the target XML document is required to conform to. The need for DTD-conformance is evident in real-life data exchange: enterprises agree on a common DTD and then exchange and interpret their XML data based on this predefined DTD.

Example 6.1: Consider the XML-to-XML transformation of promotional data for a car sale. The source data is specified by the DTD D^s_{sale} depicted in Fig. 6.1(a), in which '$*$' indicates one or more occurrences. It consists of `cars` promoted and their `features`. Each `feature` is identified by a `fid`, a key of the feature, and may be composed of other features. To exchange the data, one wants to convert the source data to a target document conforming to the DTD D_{sale} given in Fig. 6.1(c) (we omit the definition of elements of PCDATAs type). The target DTD groups `features` under each car for `sale`, along with the composition hierarchy of each `feature`. Observe that the target DTD is recursive: the element type `features` is indirectly defined in terms of itself.

As another example, consider a view for car dealers. Each dealer maintains a local



(a) DTD graph for D^s_{sale}



(b) DTD graph for D^s_{dealer}

```
<!ELEMENT promotion (sale*)
<!ELEMENT sale (make, model,
                features)
<!ELEMENT features (feature*)
<!ELEMENT feature (desc,
                features)
```

(c) Target DTD D_{sale}

```
<!ELEMENT dealer (name,
                address, cars)>
<!ELEMENT cars (car*)
<!ELEMENT car (make, model,
                price, inStock)
<!ELEMENT inStock (yes | no)
```

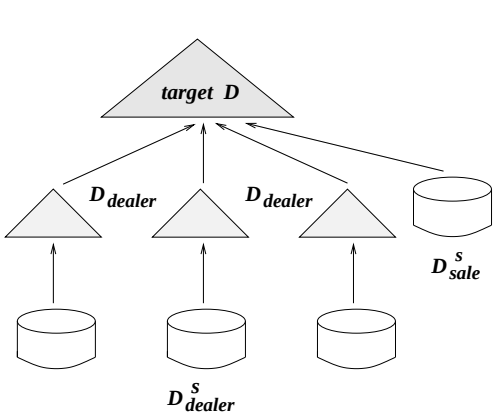
(d) Target DTD D_{dealer}

Figure 6.1: Example: Car sale and car dealers

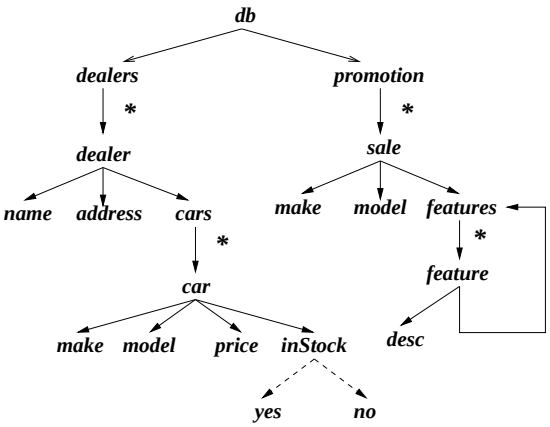
XML document specified by a source DTD D^s_{dealer}, which describes the dealer, cars carried by the dealer, and invoice, as depicted in Fig. 6.1(b). Some information is confidential, such as `invoice` and `quantity`, as indicated by the shadowed nodes in Fig. 6.1(b), which should not be made public. To hide the confidential data, one wants to define a view for each dealer such that the dealer data can only be accessed through the view. As a user interface the dealers want to provide the view DTD D_{dealer} given in Fig. 6.1(d) and requires the views to conform to D_{dealer}. Here the `inStock` status of a `car` is `yes` if its `quantity` in the original document is no less than 1; this disjunction in the target DTD leads to a non-deterministic structure.

□

Ensuring the conformance of an integrated XML document (created through multiple XML data sources) to a predefined target DTD is a non-trivial problem. First, note that the



(a) Regional integration



(b) Target DTD graph

```
<!ELEMENT db (dealers, promotion)>
<!ELEMENT dealers (dealer*)
<!ELEMENT dealer . . .    /* the same as defined by D_dealer*/
<!ELEMENT promotion . . .    /* the same as defined by D_sale*/
```

(c) Target DTD D

Figure 6.2: Example: XML integration

target DTD itself may specify a fairly complex schema structure, for example, recursive and/or non-deterministic with disjunctions. Second, the integration task may be large-scale and naturally "hierarchical" – in other words, the integration may involve a large number of distributed data sources, where some of the sources are virtual, in the sense that they are themselves views that need to be created via XML integration. This latter requirement clearly suggests that effective XML-integration specifications should be *composable*, such that large, complex integration tasks can be built via composition of simpler integration sub-tasks. This is along the same lines as modularity in programming-language principles – the key idea is to divide a complex task into manageable sub-tasks and conquer each sub-task separately.

Example 6.2: Let us consider integration of XML data for car dealers in a region together with sale promotion data. The regional integration is to extract data from XML sources and construct a single target document that consists of `sale` data, information of all the

`dealers` in the region, and `cars` carried by these dealers and promoted by `sale`. As shown in Fig. 6.2(a), the XML sources include (1) a `sale` document conforming to DTD D^s_{sale}, and (2) `dealer` views conforming to D_{dealer}, as described in Example 6.1. The target document is required to conform to the DTD D given in Fig. 6.2(c). Specifically, the integration is to transform the `sale` source data to D_{sale}, and collect `dealer` information from the views; for each dealer, it only gathers data for `cars` that are promoted by `sale`.

This integration task is rather complex. First, the target DTD is recursive and non-deterministic; its DTD graph (Fig. 6.2(b)) is cyclic and contains dashed edges (dashed edges are used to denote disjunction to distinguish from solid edges for concatenation). Second, the integration is "hierarchical": it involves a number of XML views distributed across the dealers' sites, which are in turn the result of transformation from local documents conforming to D^s_{dealer}. These views serve not only as data sources for the regional integration, but also as independent user interfaces for the dealers. Third, there is dependency on different parts of the target document: the generation of `cars` under `dealers` depends on `promotion`. Putting these in a single integration specification makes it hard to design, read and verify the correctness of the specification. □

Why not Use XQuery or XSLT? Obviously, a straightforward solution to DTD-directed XML data integration would be to employ some well-known XML query language (e.g.XQuery [Cha07], XSLT [Cla99]) to define an integrated XML view, and then check whether the resulting view conforms to the prescribed DTD. Unfortunately, such an obvious approach quickly runs into a number of technical difficulties. First and foremost, using full XML query languages to define an integrated view *cannot guarantee* DTD-*conformance*. Specifically, type inference for such derived XML views is too expensive to be used in practice: it is intractable for extremely restricted view definitions, and undecidable for realistic views [AMN+01b]. Similarly, accurate XML type checking is a hard problem – thus, languages such as XQuery typically implement only approximate type checking. Worse still, such an approach provides no guidance whatsoever on how to specify a DTD-conforming XML view. This means that DTD-directed integration becomes a trial-and-error process where, if a resulting view fails to type-check, the view definition needs to be modified and the type-checking process must be repeated. For complex integration mappings, reaching a DTD-conforming integrated view through repeated trial-and-error can be a very long and

arduous process. Second, while Turing-Complete XML query languages (such as XQuery) can express very complex integration mappings, optimization for such languages still remains to be explored, and their complexity makes it desirable to work within a more limited formalism. That is, when it comes to large-scale XML data integration, it is often desirable to trade excessive expressive power for efficiency and ease-of-use.

In this chapter, a novel formalism, XML *Integration Grammars* (XIG*s*), for the modular specification of complex, DTD-directed XML integration tasks is proposed. More concretely the key contributions of the work are summarized as follows.

• **Introduction of XIGs: The First Composable Specification Language to Support Complex, DTD-Directed XML Integration.** XIG formalism represents the first effort for modular, DTD-directed XML integration, by incorporating tree attribution, XQuery, and embedded local/remote XIG calls. In a nutshell, XIGs are built using *localized semantic rules* around productions in the target DTD which can comprise (1) *queries* over the XML sources expressed in a fragment of the XQuery language, and (2) *embedded* XIG *calls* which can be either local (i.e. executed at the same site) or remote (i.e. executed remotely). The XIG semantic rules guarantee DTD-conformance by constructing *tree-valued attributes* following the target DTD productions. XIGs are also *composable*: local/remote XIGs can be treated as "black-box" functions returning DTD-conforming XML trees, and can be embedded in an XIG definition in order to compute certain tree-valued attributes. Thus, XIGs support modular specifications of XML integration, with benefits including ease of specification/verification and reusable code.

Note that XIG formalism is *not* yet another XML transformation language; instead, XIGs are to serve as a *user/application-level interface* for specifying DTD-directed integration in XQuery. XIGs provide *guidance* on how to specify XML integration in a manner that automatically guarantees DTD conformance. Furthermore, XIGs rely on semantic rules that are *local* to each DTD production, thereby allowing integration sub-tasks to be declaratively specified for each production in isolation – this allows XIGs to simplify a complex integration task by breaking it into *small, production/element-specific pieces* that can be specified independently. XIG definitions rely solely on DTDs and XQuery, and there is no need to study any new, specialized integration language. Moreover, XIGs can be defined using some specific XQuery fragment that allows for more optimizations than full-fledged

XQuery, and, thus, can promise better performance.

• XIG**-Based Sub-framework for** DTD**-Directed Integration, Incorporating Novel, Efficient** XIG**-Evaluation Algorithms.** In CLINSE, based on XIG formalism, a middleware sub-framework for DTD-directed XML integration, along with algorithms for efficiently evaluating XIGs are proposed. Note that, in principle, it may be possible to translate any XIG into an XQuery expression and evaluate it using an XQuery-execution engine; however, taking a middleware-based approach to XIG evaluation allows us to devise several effective, XIG-specific optimization techniques that can be applied outside the generic XQuery engine. More specifically, this chapter demonstrates how to capture recursive DTDs and recursive XIGs in a uniform framework, and proposes a cost-based algorithm for scheduling local XML queries/XIGs and remote XIGs to maximize parallelism. CLINSE also provides an algorithm for merging multiple XQuery expressions into a single query without using "outer-union/outer-join". Combined with possible optimization techniques for the XQuery fragment used in XIG definitions, such optimizations can yield efficient evaluation strategies for DTD-directed XML integration.

• **Preliminary Results from a Prototype System Validating the Approach.** A prototype middleware system has been implemented for DTD-directed XML integration based on the XIG formalism and algorithms. The prototype is built on top of the Galax XQuery engine (`db.bell-labs.com/galax`) and has been tested with several synthetic XML data sets. The experimental results validate the proposed approach, clearly demonstrating the effectiveness of the XIG query-merging optimizations. Another set of experiments based on randomly-generated XIG query-dependency graphs verifies the effectiveness of the XIG-scheduling strategies.

XIGs are a first, yet concrete, step toward XML integration directed by XML Schema [Tho01]. The ultimate goal is to provide a design tool for XQuery to facilitate schema-directed integration of XML data, validating constraints in parallel with DTD-directed XML document generation in a uniform framework (note that runtime constraint/DTD checking is quite different from static analysis of consistency of XML Schema). The notion of XIGs is inspired by composable [FMY92] and higher-order [SV91] attribute grammars, which have proved useful in compiler construction. XIGs are not mild extensions of those formalisms: their definitions and evaluations are very different. Among other

things, the attribute grammar formalisms are to parse an input string with a source context-free grammar and then compute attributes associated with the parse tree; in contrast, XIGs are to generate an XML tree directed by a target DTD; the target XML tree is computed via queries in a fragment of XQuery rather than syntactic parsing.

6.1 XML Integration Grammars (XIGs)

XQuery. XIGs can be defined with any fragment of XQuery that supports FLWR constructs [Cha07] and permits effective optimization. Specifications of XML integration typically do not need a Turing-Complete language. The trade-off for the expressive power of the full-fledged XQuery is to leverage techniques for optimization and termination analyses that are not applicable to Turing-Complete languages, and to efficiently conduct XML integration tasks commonly found in practice.

Given a fragment of XQuery, its syntax is extended by incorporating XIG calls in the top level `let` clauses. Specifically, this chapter considers the class of queries defined as follows:

$$Q ::= q \mid let\ \$x := xig\_call\ Q,\ xig\_call ::= V{:}G(U) \mid G(U)$$

where q is a query in the fragment, G is an XIG, V is the URI of G (for remote XIG), and U is the URI of a source XML document. Here $V{:}G(U)$ denotes a remote XIG call, and $G(U)$ is a local XIG call. The semantics of a query "*let* $\$x := xig\_call\ Q$" is to first evaluate the XIG, assign the result of the evaluation to \$x as a constant, and then evaluate the XQuery expression q. This extension is referred to as XQs. As will be seen shortly, an XIG is defined with a target DTD D and is evaluated to an XML document of D; thus the XIG can be viewed as an XML expression of "type" D.

As will be seen in Sec. 6.3, although theoretically any XIG can be translated to an XQuery function and be evaluated using an XQuery-execution engine, there are performance reasons for not doing this.

XIG Syntax. An XIG G is a partial function from a collection X of XML sources to documents of a target DTD D, referred to as *an* XIG *from* X *to* D and denoted by $G : X \to D$.

Specifically, following the definition of DTD in Section 5.2, let $D = (Ele, P, r)$; then, G is defined on top of D as follows.

- *Attributes:* For each element type A in Ele, G defines an *inherited* attribute $Inh(\mathtt{A})$ and a *synthesized* attribute $Syn(\mathtt{A})$, whose values are a single XML element. Inherited attributes are computed top-down and are used to pass data parameter, whereas synthesized attributes are computed bottom-up and are used to hold partial results (XML subtrees).
- *Rules:* For each production $p = A \to \alpha$ in P, G defines a set $rule(p)$ of semantic rules consisting of: (1) for each child type B in α, a rule for computing $Inh(\mathtt{B})$ by extracting data from sources via an XQs query, which may take the parent $Inh(\mathtt{A})$ as a parameter; and, (2) for the parent type A, a rule for $Syn(\mathtt{A})$ by grouping together $Syn(\mathtt{B})$ for all B in α.
- *Input/Output:* The sources X is called the *input* of G, the value of the synthesized attribute $Syn(\mathtt{r})$ of the root is the *output* of G, and D is the *type* of G.

Given an input X, $G(X)$ returns $Syn(\mathtt{r})$, which is an XML document conforming to the target DTD D.

Example 6.3: Fig. 6.3 gives an XIG that defines a view for local dealers: given the URI U of a local document specified by the DTD D^s_{dealer} of Fig. 6.1(b), $G_{dealer}(U)$ returns an XML document conforming to D_{dealer} of Fig. 6.1(d). Thus G_{dealer} can be treated as a function: $D^s_{dealer} \to D_{dealer}$. The XIG is defined on top of the (target) view DTD D_{dealer} with XQs queries and tree attribution. For each element type A in D_{dealer}, it defines two attributes $Inh(\mathtt{A})$ and $Syn(\mathtt{A})$, which contain a single XML element as their value. For each production of D_{dealer}, it defines a set of rules via XQs to compute the inherited attributes of the children, using the inherited attribute of the parent as a parameter. In addition, there is a single rule for computing the synthesized attribute of the parent, by collecting the synthesized attributes of its children. □

For a production $p = A \to \alpha$, the semantic rules $rule(p)$ enforce that $Syn(\mathtt{A})$ is indeed an A element. The generic form of the (per-production) XIG semantic rules is as follows.

• $p = A \to \mathsf{str}$. Then, $rule(p)$ is defined as $Syn(\mathtt{A}) = \{Q(Inh(\mathtt{A}))/text()\}$, where Q is an XQs query that returns PCDATAs and treats $Inh(\mathtt{A})$ as a constant parameter. See, e.g. the

XIG: $G_{dealer}(U)$

dealer → name, address, cars

Inh(name)= {U/dealer/name}; *Inh*(address) = {U/dealer/addr};
Inh(cars) = {U/dealer/cars};
Syn(dealer) = <dealer> {*Syn*(name)} {*Syn*(address)}
{*Syn*(cars)} </dealer>

cars → car*

Inh(car) ← for $c in *Inh*(cars)/car return $c;
Syn(cars) = <cars> {⊔*Syn*(car)} </cars>

car → make, model, price, inStock

Inh(make) = {*Inh*(car)/make}; *Inh*(model) = {*Inh*(car)/model};
Inh(price) = {*Inh*(car)/invoice/price}; *Inh*(inStock) = {*Inh*(car)};
Syn(car) = <car> {*Syn*(make)} {*Syn*(model)}
{*Syn*(price)} {*Syn*(inStock)} </car>

inStock → (yes + no)

Inh(yes) = {if *Inh*(inStock)[invoice/quantity < 1]
then <empty/> else <yes/>}
Inh(no) = {if *Inh*(inStock)[invoice/quantity < 1]
then <no/> else <empty/>}
Syn(inStock) = {if *Inh*(inStock)[invoice/quantity < 1]
then *Syn*(no) else *Syn*(yes)}

yes → ε

Syn(yes) = *Inh*(yes) /* similarly for **no** */

name → PCDATA

Syn(name) = <name> {*Inh*(name)/text()} </name>
/* similarly for **address, make, model, price** */

Figure 6.3: XIG $G_{dealer}(U)$ defining dealer views

rule for production *name* → PCDATA*s* in the XIG G_{dealer} of Fig. 6.3.

• $p = A \rightarrow B_1, \ldots, B_n$. Then, $rule(p)$ consists of $Inh(\texttt{B}_\texttt{i}) = \ Q_i(Inh(\texttt{A}))$, for each $i \in [1,n]$, and $Syn(\texttt{A}) =$ <A> $\{Syn(\texttt{B}_1) \ldots \ Syn(\texttt{B}_\texttt{n})\}$</A>, where, for each $i \in [1,n]$, Q_i is an XQs query that returns a single element (subtree). As an example, see the rules for *car* → *make, model, price, inStock* in G_{dealer}.

• $p = A \rightarrow B_1 + \ldots + B_n$. Then $rule(p)$ is defined as:

$Inh(\texttt{B}_\texttt{i})$ = **let** \$c := $Q_c(Inh(\texttt{A}))$ **return** {**if** C_i(\$c) **then** $Q_i(Inh(\texttt{A}))$

else <empty/>} /* for $i \in [1,n]$*/,

$Syn(\texttt{A})$ = **let** \$c := $Q_c(Inh(\texttt{A}))$ **return**
{if C_1(\$c) **then** <A> $Syn(\texttt{B}_1)$ </A> **else** . . .

else if C_n(\$c) **then** <A> $Syn(\texttt{B}_\texttt{n})$ </A> **else** <empty/>}

where Q_c is an XQs query, referred to as the *condition query* of $rule(p)$, which is evaluated only once for all the rules in $rule(p)$; Q_i is an XQs query that returns a single element; and, the C_i's are *mutually-exclusive* Boolean XQs expressions: one and only one C_i is true for all $i \in [1,n]$. See, e.g. the rules for the production *inStock* → *yes + no* in G_{dealer}.

• $p = A \rightarrow B^*$. Then, $rule(p)$ is defined as:

$Inh(\texttt{B})$ ← **for** \$b **in** $Q(Inh(\texttt{A}))$ **where** C(\$b) **return** \$b,

and $Syn(\texttt{A}) =$ <A> $\sqcup Syn(\texttt{B})$ </A>, where Q is an XQs query that may return a (possibly empty) set of elements, C is an XQs Boolean expression, and '$\sqcup$' is a list constructor. For each \$*b* generated by Q, the rules for processing B are evaluated, treating \$*b* as a value of $Inh(\texttt{B})$. Then, the rule for $Syn(\texttt{A})$ groups together the corresponding $Syn(\texttt{B})$'s into a list using $\sqcup$ in the default document order. See, e.g. the rules for *cars* → *car** in G_{dealer}.

• $p = A \rightarrow \varepsilon$. Then, $rule(p)$ is defined as $Syn(\texttt{A}) = Q(Inh(\texttt{A}))$, where Q is an XQs query such that $Q(Inh(\texttt{A}))$ returns either <A/>, or <empty/> if the value of $Syn(\texttt{A})$ is not to be included in the target document. See, e.g. the rule for *yes* → ε in G_{dealer}.

Several subtleties are worth mentioning. First, recall that $Syn(\mathtt{A})$ is defined in terms of $Syn(\mathtt{B_i})$. In the rule for computing $Syn(\mathtt{A})$ one may replace $Syn(\mathtt{B_i})$ with the XQs query for computing $Syn(\mathtt{B_i})$ (defined in the rules for B_i). For example, in the XIG G_{dealer}, the rules for `dealer` and `car` can be rewritten as:

dealer → name, address, cars

Inh(cars) = {U/dealer/cars};
Syn(dealer) = <dealer> {U/dealer/name}
{U/dealer/addr} {*Syn*(cars)} </dealer>

car → make, model, price, inStock

Inh(inStock) = {*Inh*(car)};
Syn(car) = <car>{*Inh*(car)/model} {*Inh*(car)/make}
{*Inh*(car)/invoice/price} {*Syn*(inStock)}</car>

These substitutions can avoid unnecessary computation of inherited attributes that are not needed elsewhere. Second, as XIGs support tree attribution and return XML trees, semantic attributes can be computed via other XIGs; such an example will be given in the rule for $Syn(\mathtt{promotion})$ in the XIG G of Fig. 6.5. Furthermore, as embedded XIGs ensure conformance to their target DTDs, one can use them as expressions without complicating the typing analyses. This makes XIGs composable.

XIG Semantics. We next give a simple operational semantics for an XIG $G : X \to D$. Given an instance of X, G evaluates its attributes via its rules, and returns $Syn(\mathtt{r})$ of the root r of D as its output. The evaluation is carried out top-down, using a stack. The root r is first pushed onto the stack. For each node A at the top of the stack, we compute its subtree $Syn(\mathtt{A})$. To do this, we first identify the production $p = A \to \alpha$ in D, and for each B in α, we evaluate $Inh(\mathtt{B})$ using the semantic rules in $rule(p)$. The exact procedure depends on the specific form of the p production. For example, if $p = A \to B_1, \ldots, B_n$, then for each B_i, we compute $Inh(\mathtt{B_i})$ by evaluating $Q_i(Inh(\mathtt{A}))$; we then push B_i onto the stack and proceed to process them in the same way using the value of $Inh(\mathtt{B_i})$; then, after all the B_i's are evaluated and popped off the stack (i.e. when all the $Syn(\mathtt{B_i})$'s are available), we compute $Syn(\mathtt{A})$ by collecting all the $Syn(\mathtt{B_i})$'s, such that A has a unique B_i child for each

$i \in [1,n]$. (The process for other production rules is similar; due to space constraints, we defer the details to the full paper.) Finally, after $Syn(\mathtt{A})$ is computed, we pop A off the stack, and use $Syn(\mathtt{A})$ to evaluate other nodes until no more nodes are in the stack. At this stage, $Syn(\mathtt{r})$ is computed and returned as the output of the XIG evaluation. Note that for each A, its inherited attribute is evaluated first, then its synthesized attribute, which is an A-subtree. The evaluation takes *one-sweep*: each A element is visited twice, first pushed onto the stack and then popped off after its subtree is constructed. It should be mentioned the conceptual evaluation strategy given above is just to illustrate the semantics of XIGs; we shall provide optimization techniques in Section 7.7.

6.2 Case Study

To illustrate the idea of DTD-directed integration with XIGs, consider the integration described in Example 6.2. The regional integration is to extract data from dealer views and a sale document, and construct a target document conforming to the target DTD D of Fig. 6.2(c), where the dealer views are themselves mapped from local sources at dealer's sites. We divide this task into three parts, and specify each with an XIG as follows.

- $G_{dealer} : D^s_{dealer} \rightarrow D_{dealer}$ is the XIG of Fig. 6.3 that defines a view for dealers: given the URI U of a local document specified by the DTD D^s_{dealer} of Fig. 6.1(b), $G_{dealer}(U)$ returns an XML document conforming to D_{dealer} of Fig. 6.1(d). Each local dealer has a G_{dealer} residing at its site and serving as a view. While the view DTD D_{dealer} is visible to the users, the source DTD D^s_{dealer} and the definition of G_{dealer} are not. The view does not reveal confidential information about `invoice` and `quantity`.
- $G_{sale} : D^s_{sale} \rightarrow D_{sale}$ is an XIG that converts sale data: given the URI X of a sale document specified by D^s_{sale} of Fig. 6.1(a), $G_{sale}(X)$ returns an XML document conforming to the DTD D_{sale} of Fig. 6.1(c). This XIG G_{sale} is local: it is at the integration site.
- G is an XIG for regional integration: it is defined with G_{dealer} as a remote XIG and G_{sale} as a local XIG. It takes as input the URI X of the sale source and an XML file R containing information for dealers in the region. Specifically, R consists of a sequence of `dl`'s, and each `dl` is of the form (V,U), where V is the URI of G_{dealer}

XIG: $G_{sale}(X)$

promotion → **sale***

Inh(sale) ← for $c in X/sale/cars/car return $c;

Syn(promotion) = <promotion>{⊔*Syn*(sale)}</promotion>

sale → **make, model, features**

Inh(make)={*Inh*(sale)/make}; *Inh*(model)={*Inh*(sale)/model};

Inh(features) = {*Inh*(sale)/fids};

Syn(sale) = <sale> {*Syn*(make)} {*Syn*(model)}
{*Syn*(features)} </sale>

features → **feature***

Inh(feature) ← for $f in *Inh*(features)/fid return $f;

Syn(features) = <features>{⊔*Syn*(feature)}</features>

feature → **desc, features**

Inh(desc)=X/sale/features/feature[fid=*Inh*(feature)]/desc;

Inh(features)=X/sale/features/feature[fid=*Inh*(feature)]/fids;

Syn(feature)=<feature>{*Syn*(desc)}{*Syn*(features)}</feature>

make → **PCDATA** /* similarly for **model, desc** */

Syn(make) = {*Inh*(make)}

Figure 6.4: XIG $G_{sale}(X)$ for converting sale data

and U is the URI of the local source data at the same dealer site[1]. The XIG G invokes $G_{sale}(X)$ and $V : G_{dealer}(U)$ for each (V,U) to collect data from dealer sources and then constructs an XML document conforming to the target DTD of Fig. 6.2(c).

We have already seen the XIG G_{dealer} in Fig. 6.3. We next present G_{sale} and G.

Sale Data. An XIG $G_{sale} : D^s_{sale} \to D_{sale}$ for converting sale data is given in Fig. 6.4. Given a source X, $G_{sale}(X)$ is evaluated top-down. Starting from `promotion`, it uses an XQs query to extract `car` elements from X, and treats each `car` $\$c$ as a value of *Inh*(`sale`).

[1]Assume that the definition of G_{dealer} is not accessible to anyone except the dealer, and that the local source document is only accessible to the dealer or via G_{dealer}, although their URIs are public.

For each $\$c$ the rules for `sale` are evaluated, which compute *Inh*(`make`), *Inh*(`model`) and *Inh*(`features`) by extracting the corresponding fields from $\$c$, and invoke the rules for `features` in turn. Note that `features` is recursively defined and thus its subtree has an unbounded depth. The depth is determined at run time: if the XQs query for computing *Inh*(`feature`) does not find any `fid`, the rules for computing `feature` subtree are not triggered, the list $\sqcup$*Syn*(`feature`) is empty, and the construction of `features` subtree is complete. After all the subtrees *Syn*(`features`) are constructed, *Syn*(`sale`) is computed, followed by *Syn*(`promotion`). This example shows that XIGs are capable of expressing XML integration with a recursive target DTD.

It is important to note here that XIGs adopt a *data-driven semantics*: the height of the XML tree in the recursive case and the choice of a production in the non-deterministic case are determined by queries on the XML source data at run-time.

Regional Integration. Finally, we provide an XIG G in Fig. 6.5 for integrating XML data of car dealers and promotion information. It is defined with embedded XIGs: local XIG G_{sale} and remote XIGs G_{dealer}. The local XIG G_{sale} is invoked to produce *Syn*(`promotion`), which is an XML tree conforming to the `promotion` type of the target DTD D. To produce *Syn*(`dealers`), it first finds from the input document R the URI $\$v$ of the view G_{dealer} and the URI $\$u$ of the local dealer source for each dealer. For each pair ($\$v, $\$u), it then invokes the remote XIG G_{dealer} via $\$v{:}G_{dealer}(\$u)$ to compute its view. The result of the computation, $\$p$, is shipped back to the integration site and is used as a constant in the queries for computing *Inh*(`name`), *Inh*(`address`) and *Inh*(`cars`). To find the cars that are promoted, i.e. those appearing in $G_{sale}(X)$, G invokes $G_{sale}(X)$ and selects cars that are in both $\$p$ and $G_{sale}(X)$. For each car $\$c$ selected, it simply returns $\$c$ as *Syn*(`car`), since G_{dealer} ensures that $\$c$ indeed conforms to the `car` type in the target DTD D. This example shows how a complex integration task can be carried out in terms of component XIGs.

6.3 XML Integration Sub-framework

A middleware-based sub-framework for XIG evaluation has been proposed in CLINSE. As shown in Fig. 6.6(a), the middleware takes an XIG G as an input, evaluates G and generates an XML document conforming to the target DTD of G. More specifically, the XIG middle-

XIG: $G(R,X)$

db → dealers, promotion

Syn(db) = <db> {Syn(dealers)} {Syn(promotion)} </db>

promotion → sale*

Syn(promotion) = $V_{sale}(X)$

dealers → dealer*

Inh(dealer) = for $Y in R/dl return $Y;

Syn(dealers) = <dealers>{⊔Syn(dealer)}</dealers>

dealer → name, address, cars

Inh(name) = let $v := Inh(dealer)/V /* similarly for */
let $u := Inh(dealer)/U /* address, cars */
let $p = $v:$G_{dealer}$($u)
return $p/dealer/name;

Syn(dealer) = <dealer> {Syn(name)} {Syn(address)}
{Syn(cars)} </dealer>

cars → car*

Inh(car) ← let $s := $G_{sale}(X)$
for $c in Inh(cars)/car
$c′ in $s/promotion/sale
where $c/make=$c′/make and $c/model=$c′/model
return $c;

Syn(cars) = <cars> {⊔Syn(car)} </cars>

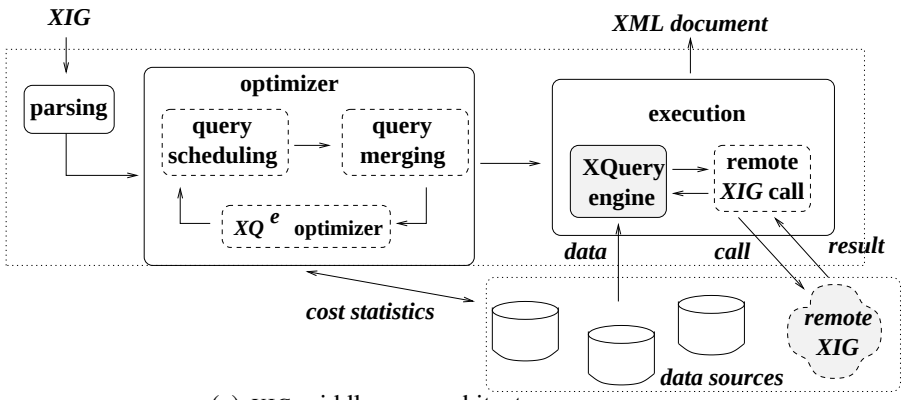
car → make, model, price, inStock

Syn(car) = Inh(car)

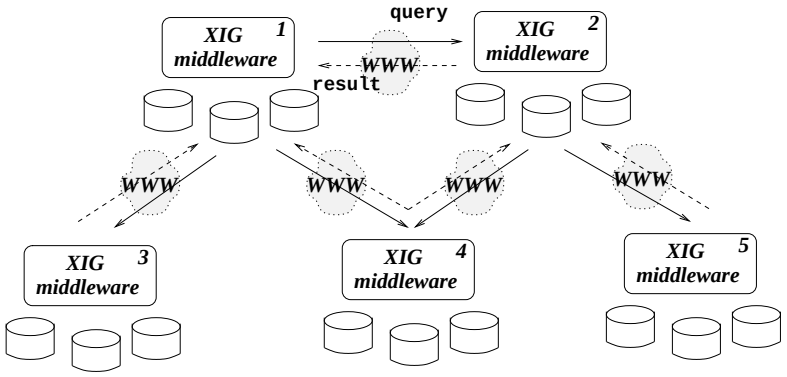
name → PCDATA /* similarly for address */

Syn(name) = Inh(name);

Figure 6.5: XIG $G(R,X)$ for regional integration



(a) XIG middleware architecture



(b) XIG middleware communication

Figure 6.6: XIG-based sub-framework for DTD-directed integration

ware servers use a local XQuery engine to evaluate XQs queries over local data sources. An XIG server also communicates with other servers. It invokes a remote XIG G' along the same lines as a *remote procedure call*: it sends a request along with appropriate data parameters to the server where G' is located; the remote server then evaluates G' and sends the result back. Note that a remote XIG may in turn invoke XIGs at other servers. For example, as depicted in Fig. 6.6(b), server 1 invokes remote XIGs at servers 2, 3 and 4, and to evaluate the remote XIG call of server 1, server 2 in turn invokes XIGs at servers 4 and 5.

Note that, although theoretically one can translate an XIG specification of a complex integration task into a large XQuery function (by simply *merging* the localized semantic rules for all DTD productions) when there is only a single source, such brute force query merging typically leads to poor performance in practice. First, injudicious query merging relies on the optimizer of the underlying XQuery-engine to optimize a large query, sched-

ule execution of queries and XIGs, and produce efficient execution plans. However, even sophisticated relational optimizers do not work well on large SQL queries, not to mention XQuery optimizers that remain to be explored. Indeed, injudicious query-merging has proved ineffective in relational publishing/integration practice, and this was one of the main motivations for developing middleware systems and appropriate optimization techniques [BCF+03, BCF+02, BGK+02, FMS01, Sha99]. Second, it is possible to develop optimization techniques that are effective for the specific XQs fragment used in XIGs but are not applicable to XQuery in general and are unlikely to be supported inside a generic XQuery engine. This suggests that potential optimizations developed for XQs fragment should probably be accommodated in the middleware server (outside the XQuery engine). Third, brute force query merging is actually an extreme case in our cost-based query scheduling and merging. If brute-force merging is the best plan, it will be automatically selected by our cost-based optimizer. However, in our experiments, this is rarely the case. When multiple sources are involved in the integration, it is not possible to merge the queries on different sources since current XQuery specification [Cha07] has not yet defined remote procedure calls.

Thus, central to the XIG middleware is an XIG *optimizer* module (Fig. 6.6(a)) whose goal is to generate an efficient execution plan that minimizes the response time of an XIG evaluation. After an initial parsing phase, which derives the dependency relation on the queries of the input XIG G, the XIG optimizer generates an execution plan for G using a cost-based approach that: (1) merges certain queries in G that are processed at the same source into a larger query to reduce communication costs, (2) schedules execution of XQs queries and XIGs to increase parallelism, and (3) leverages an external optimizer for (partially-merged) XQs queries to produce efficient XQs-execution plans. Finally, the execution plan is carried out, by evaluating optimized (merged) XQs queries embedded in G via a local XQuery engine, and by invoking remote XIG calls. Compared to its counterparts for XML publishing [BCF+02, CFI+00, FMS01] and relational data integration in XML [BCF+03], the XIG optimizer raises a number of new issues that will be briefly addressed below; detailed optimization algorithms are provided in Section 7.7.

XIG **Recursion vs.** DTD **Recursion.** This XIG-based integration sub-framework involves two forms of recursion: recursive target DTDs and recursive XIGs (i.e.XIGs defined in terms

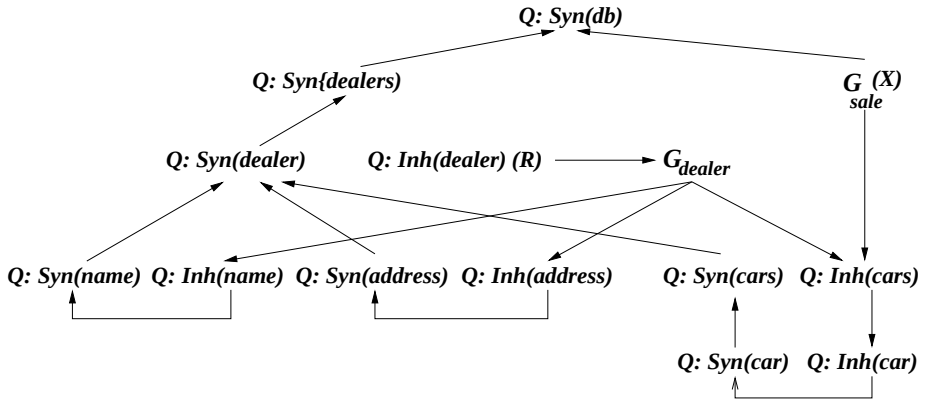
of themselves). In contrast, previous work on XML integration/publishing either ignores recursion or considers recursive DTDs only [BCF+02, BCF+03].

The key observation here is that recursive DTDs can be captured with recursive XIGs. Indeed, the computation of any recursively-defined A-elements can be rewritten to an equivalent local, recursive XIG G_A. For example, we can easily define a recursive XIG for computing the recursively-defined `features` elements in Fig. 6.4. The rewriting is conducted in the parsing phase of the XIG middleware of Fig. 6.6(a). This allows us to handle the two forms of recursion in a uniform framework.

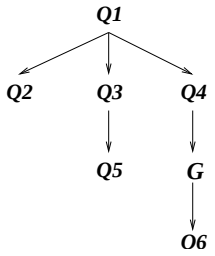
Recursive XIG evaluation also raises *termination* issues. To avoid potential infinite invocation loops, the XIG middleware servers employ a dynamic control mechanism based on keeping track of local XIG invocations and using that information to detect cycles in the call chain. Furthermore, XIG servers also cache the results of XIG evaluations to avoid possible redundant computation.

Data shipping vs. query shipping. For a query over a remote data source, XIG middleware may either bring the data over to the server and evaluate the query with its local XQuery engine, or ship the query to the remote site, evaluate the query on that site and then ship the result back. The decision of *query shipping vs. data shipping* is based on their respective costs, which involve communication cost, query execution overhead and workload of related servers. For example, to evaluate the local XIG $G_{sale}(X)$ embedded in the XIG G of Fig. 6.5, it may be more efficient to bring the data file X over than to ship the queries of $G_{sale}(X)$ to the remote site, since, among other things, the result of $G_{sale}(X)$ contains the transitive closure of `feature` in X and may be larger than the original X file. In contrast, the middleware systems of [BCF+02, BCF+03] always ship query to data sources.

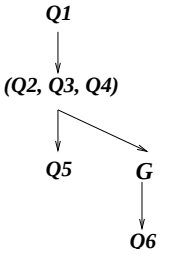
Query Dependencies. XIGs support sideways information passing in an implicit way: common computation is specified with an XIG, which is invoked wherever it is needed. For example, the XIG G of Fig. 6.5 uses G_{sale} to specify the computation of the `promotion` subtree, and invokes G_{sale} at two different places where the subtree is needed. This yields a more flexible information passing mechanism than other proposals, e.g. data passing between siblings [BCF+03]. However, naive evaluation of G may lead to repeated evaluation of G_{sale}. To eliminate unnecessary XIG re-computation, the system explicitly captures the dependencies among XIG queries through a *query dependency graph*.



(a) The query dependency graph of G



(b) Query dependency



(c) Query merging

Figure 6.7: Query dependency, scheduling and merging

The *query dependency graph* of an XIG G contains a node for each query/XIG in G, and a directed edge from Q_1 to Q_2 if and only if the result of Q_1 is consumed by Q_2. For example, the dependency graph of the XIG G of Fig. 6.5 is depicted in Fig. 6.7(a), in which $Q : Inh(\mathtt{A})$ and $Q : Syn(\mathtt{A})$ denote the queries for computing $Inh(\mathtt{A})$ and $Syn(\mathtt{A})$, respectively. The graph describes top-down dependencies on inherited attributes, bottom-up dependencies on synthesized attributes, and producer-consumer relationships introduced by embedded (local and remote) XIGs. Note that there is a single node representing the XIG G_{sale}, which is evaluated once and its result is used to compute both $Syn(\mathtt{db})$ and $Inh(\mathtt{car})$. Also, note that, once recursively-defined elements are rewritten as recursive XIGs (XQs functions), the parsing phase of the middleware inspects whether the query dependency graph is cyclic and allows only *directed, acyclic graph (DAG)*. (Cyclic dependency graphs are infeasible and are rejected.)

Query Scheduling. Based on the query dependencies in an XIG, the XIG-middleware optimizer orders the execution of queries/XIGs such that local queries and remote XIGs can be evaluated in parallel. For example, consider the dependency of Fig. 6.7(b), where $Q_1, \ldots, Q_6$ are local queries and G is a remote XIG call. One may want to execute Q_4 before Q_2 and Q_3 such that G can be evaluated by another server in parallel with Q_2, Q_3, and thus improve the overall response time. It is, however, nontrivial to develop an optimal scheduling strategy. Among other things, XIGs are complex tasks and a remote XIG may trigger other remote XIGs. For example, referring to Fig. 6.6(b), server 1 triggers remote XIGs at servers 2 and 4, while the remote XIG at server 2 may invoke another XIG at server 4, competing for the resources of server 4.

Query Merging. Another optimization technique is to *merge* multiple XQs queries into a single query. For example, an XIG without remote XIG calls can be easily rewritten as a single XQs query. The merged XQs queries can then be optimized via an XQs optimizer (Fig. 6.6(a)). Query merging could reduce the communication overhead between the middleware and the underlying XQuery engine, and thus potentially speed up the query execution. On the other hand, injudicious query merging may change the query dependency graph, lead to unnecessary delay of other query executions, and decrease parallelism. For example, merging Q_2, Q_3, Q_4 of Fig. 6.7(b), results in the query dependency DAG shown in Fig. 6.7(c). As a result, the remote XIG call G is delayed as it becomes dependent on Q_2 and Q_3 as well, thus decreasing the potential parallelism among remote XIGs and local queries. Clearly, the decision of whether or not to merge certain queries should be *cost-based*; furthermore, given the dependence of execution cost on scheduling, query merging and scheduling are obviously dependent on each other.

Thus one should decide whether or not to merge certain queries based on the costs. In addition, because of the interaction between query merging and scheduling, the two have to be dealt with together.

6.4 XIG Evaluation and Optimization

In this section, two cost-based algorithms are presented for scheduling and merging XQs/XIG expressions to improve the response time of XIG evaluation. These can be com-

bined with optimizations for XQs queries, i.e. the middleware is open to and can accommodate optimization techniques for specific XQuery fragments.

Scheduling an XIG Evaluation. Assume a given *query dependency DAG* that captures the data and execution dependencies between the various components (namely, XQs and XIG expressions) comprising an XIG. Note here that, although XQs queries are typically executed locally, XIG nodes can be either local or remote (i.e. with the XIG executed at a remote server). Effectively scheduling such an XIG-dependency DAG over an architecture of distributed servers is a very challenging problem. In addition to all the complications typically associated with scheduling a DAG of inter-dependent (i.e.*precedence-constrained*) tasks over a distributed architecture (e.g. communication overhead, parallel execution), a crucial, distinguishing characteristic of the problem is that XIGs are *complex tasks* that can invoke other (local or remote) XIG tasks for their evaluation. In essence, this means that, instead of simply utilizing a single server, the evaluation of an XIG node in the query dependency DAG can utilize several different servers (through embedded remote XIG calls). This strict co-scheduling requirement makes the XIG-scheduling problem quite different from those studied in the context of conventional scheduling for parallel/distributed systems, where the assumption is that either each task uses a single site [HM95] or that tasks can be migrated across different subsets of sites [BFV96, GI97].[2] Similarly, work on dynamic/adaptive scheduling strategies for distributed database and data-integration systems (e.g. [IFF+99, BFMV00]) is applicable only at run-time, that is, when the query plan is actually executed. In contrast, the focus here is on *compile-time* scheduling in order to determine an effective XIG-evaluation plan; thus, the scheduling model needs to be able to capture all the complexities of XIG evaluation.

Given an XIG query dependency graph G, determining a schedule for G over the underlying architecture of distributed servers that minimizes the overall XIG execution time (i.e. the *makespan* of the schedule) is an essential step in optimizing XIG evaluation. The scheduler needs to make its decisions at XIG-optimization time, which means that it needs to rely on estimates for query/XIG execution costs, result sizes, and communication overheads. In the implementation, we assume that each server s in the underlying system offers

[2]Note that the corresponding scheduling problem for AIG evaluation [BCF+03] also assumes only single-site queries.

a query/XIG-costing API that, given a query/XIG node t to be executed at s returns (1) an estimate $l(t)$ for the processing time of t's execution on s; and, (2) a subset of sites $S(t)$ (including s) that are utilized in the evaluation of t (where $|S(t)| > 1$, if t is an XIG node with embedded remote XIG calls).[3] Thus, for each node t in the dependency graph, the underlying server APIs provide us with the execution time of t as well as the (sub)set of servers used during this execution. The XIG-scheduling problem can then be abstracted as follows.

XIG SCHEDULING($G, \mathcal{S}, l(), S()$)

• **Given:** A dependency DAG $G = (V, E)$ defining a partial order (precedence) relation "$\prec$" over a set of tasks $V = \{t_1, \ldots, t_n\}$; set of distributed servers $\mathcal{S}$. For each task $t \in V$, $l(t)$ is the execution time of t and $S(t) \subseteq \mathcal{S}$ is the set of servers used during t's execution.

• **Find:** An assignment of start times to tasks $\mathsf{start} : V \rightarrow R^+$, such that:

1. Concurrently-executing tasks *do not collide* on servers – that is, for all $i \neq j$, if $[\mathsf{start}(t_i), \mathsf{start}(t_i) + l(t_i))] \cap [\mathsf{start}(t_j), \mathsf{start}(t_j) + l(t_j))] \neq \phi$ then $S(t_i) \cap S(t_j) = \phi$.
2. Precedence constraints are satisfied – that is, for all $t_i \prec t_j$ we have $\mathsf{start}(t_j) \geq \mathsf{start}(t_i) + l(t_i)$; and,
3. The schedule makespan $\max_i\{\mathsf{start}(t_i) + l(t_i)\}$ is *minimized*.

It is easy to verify that the XIG-scheduling problem is actually the precedence-constrained generalization of the *Set Scheduling* problem recently introduced by Goel et al. [GHPT99]. Even for their simpler case of fully-independent tasks (i.e. $\prec = \phi$), Goel et al. demonstrate that the problem is NP-hard and hard to approximate, by giving a simple, approximation-preserving reduction from the *Minimum Graph Coloring* problem [GHPT99]. Given the intractability of the XIG SCHEDULING problem, now a heuristic scheduling algorithm is proposed for query dependency graphs that produces an approximate solution to the scheduling problem.

[3] To simplify the exposition, we assume that the query/XIG-processing time $l(t)$ also includes the cost of communicating input/output data to/from the executing server s, which also allows us to leave result-size estimates out of the scheduling-problem formulation. Both aspects can be incorporated into the scheduling model and algorithms in a straightforward fashion.

In a nutshell, the scheduling algorithm (termed SCHEDXIG) belongs to the class of *list-scheduling* algorithms, originally introduced by Graham for multiprocessor scheduling [Gra69]. SCHEDXIG maintains a list L of *ready* tasks (i.e. tasks whose predecessors in the dependency graph G have already completed), and schedules the next ready task $t \in L$ at the earliest possible start time (i.e. the earliest time at which all servers in $S(t)$ become available). Since the goal is to minimize the overall execution time in the schedule for G, we maintain the tasks in the ready list L sorted in decreasing order of *"criticality"*, where the criticality of a ready task t (denoted by $\mathsf{crit}(t)$) captures t's potential in becoming the bottleneck (i.e. lie in the critical path) for the parallel execution of G. Note that estimating the criticality of a task node in the complex-task model used in the XIG-scheduling problem is non-trivial – the criticality measure needs to account not only for the serialization effects in the parallel execution (introduced by the dependency edges in G), but also for the possibility of collisions of independently-executed tasks utilizing the same server(s). The SCHEDXIG algorithm employs such a criticality measure that is a simple-to-compute lower bound $\mathsf{crit}(t)$ on the parallel-execution time of all DAG paths rooted at task node t and captures both the serialization and the server-collision effects mentioned above. More formally, let $\mathsf{paths}(t)$ denote the set of all paths rooted at task t (including t itself) and leading to some "sink" node in G, and let $G(t)$ denote the corresponding subgraph of G. Also, given a task t, define the *server-usage vector* $\mathbf{v}(t)$ of t to be a numeric vector of dimensionality $|\mathcal{S}|$ (i.e. the number of servers in the system), and components defined as: $\mathbf{v}(t)[i] = l(t)$ if $i \in S(t)$, and 0 otherwise (where we assume, w.l.o.g, that $\mathcal{S} = \{1, 2, \ldots, |\mathcal{S}|\}$). Thus, $\mathbf{v}(t)$ basically captures the processing-time requirements of t on each server used during t's execution. We estimate the criticality of t, $\mathsf{crit}(t)$, as the *maximum* of the following two quantities:

1. The *Critical-Path Length under* t, $\mathsf{CP}(t) = \max_{p \in \mathsf{paths}(t)} \{\sum_{u \in p} l(u)\}$, which captures the effects of dependencies (i.e. serialization constraints) in the parallel execution of $G(t)$; and,

2. The *Maximum Server Load under* t, $\mathsf{SL}(t) = \max_i \{\sum_{u \in G(t)} \mathbf{v}(u)[i]\}$, which captures the effects of possible server collisions and server bottlenecks during the parallel execution.

Example 6.4: Consider a simple instance of the XIG SCHEDULING problem, with 4 tasks

$V = \{t_1, \ldots, t_4\}$ and the task dependencies $t_1 \rightarrow t_2 \rightarrow t_3$, $t_1 \rightarrow t_4$. Assume a 3-server configuration, and let $\mathbf{v}(t_1) = [2,0,0]$, $\mathbf{v}(t_2) = [0,8,0]$, $\mathbf{v}(t_3) = [5,0,0]$, and $\mathbf{v}(t_4) = [0,0,10]$. It is easy to see that, in this scenario, $\mathsf{CP}(t_1) = \max\{2+8+5,\ 2+10\} = 15$ and $\mathsf{SL}(t_1) = \max\{[2+5,\ 8,\ 10]\} = 10$, which implies that $\mathsf{crit}(t) = \max\{\mathsf{CP}(t_1),\ \mathsf{SL}(t_1)\} = 15$; that is, the dominant factor in this parallel execution comes from the serialization in the $t_1 \rightarrow t_2 \rightarrow t_3$ dependency chain. In contrast, assume that t_4 is a complex (XIG) task that utilizes both servers 2 and 3, i.e. $\mathbf{v}(t_4) = [0,10,10]$. It is again easy to see that, in this case, even though the critical-path length $\mathsf{CP}(t_1)$ remains the same, the maximum server load becomes $\mathsf{SL}(t_1) = \max\{[2+5,\ 10+8,\ 10]\} = 18$, which implies that $\mathsf{crit}(t) = \mathsf{SL}(t_1) = 18$ – thus, the dominant execution-time factor has shifted to the processing bottleneck created by the collision of t_2 and t_4 on server 2. □

The pseudo-code for the SCHEDXIG algorithm is given in Fig. 6.8; its worst-case time complexity is $O(n|\mathcal{S}|\log n)$ (e.g. using a max-heap for L). Note that, even though we presented the algorithm SCHEDXIG as an optimization-time technique, it is actually an online algorithm that can readily be used to schedule XIG executions at run-time (based on task-criticality estimates) as servers become available. Finally, we should note that the complex-task model can be generalized along the lines of the *preemptable/time-shared* resource model of [GI97] to allow for servers to be effectively time-shared across different tasks, since, e.g. an XIG node can typically impose different processing requirements on the remote servers it utilizes. This gives rise to several challenging scheduling issues that we are exploring in the ongoing work.

Merging Queries. Query merging may also speed up XIG evaluation; however, it can also change the dependency DAG and, thus, the execution schedule (and corresponding evaluation cost). Thus, query merging and scheduling are clearly inter-dependent. The query merging problem is to determine, given a dependency graph G, what query nodes to merge such that the *estimated response time* of the resulting dependency graph G' (i.e. the makespan of the schedule returned by SCHEDXIG (G')) is minimized.

Given a dependency graph G, there are exponentially many choices for merging queries in G; moreover, recall that the scheduling problem is already intractable. Given the inherent difficulty of the problem, we outline a greedy heuristic algorithm, termed MERGEXIG, that iteratively calls the SCHEDXIG scheduler for optimizing XIG query merging and eval-

Procedure SCHEDXIG $(G, \mathcal{S})$
Input: XIG dependency graph G, set of servers $\mathcal{S}$.
Output: Schedule start() for executing G over $\mathcal{S}$.
begin
1. **for each** node t in G **do**
2. compute crit(t) := max{CP(t), SL(t)}
3. L := list of ready XQs/XIG tasks in G in decreasing order of crit(t)
4. **while** $L \neq \phi$ **do**
5. $t := L[1]$ /* first ready task in L*/
6. start(t) := earliest time in the schedule that all servers in $S(t)$ become available
7. M := list of tasks in G that become ready after the completion of t (in decreasing crit())
8. $L :=$ **merge**$(L - L[1], M)$
9. **endwhile**

end

Figure 6.8: The XIG-Scheduling Algorithm.

uation. In a nutshell, MERGEXIG takes an XIG dependency graph G as input and returns an efficient evaluation schedule as output. At each step, MERGEXIG considers each pair of query nodes (Q_1, Q_2) in G that are processed at the same source for potential merging into a single query node Q (resulting in a new dependency graph G'); the query pair resulting in the (acyclic) dependency graph G' with the lowest SCHEDXIG-estimated evaluation cost (i.e. the smallest makespan for SCHEDXIG (G')) is merged. The iteration in MERGEXIG continues until no further cost reduction is possible; at that time, SCHEDXIG is invoked on the final (merged) dependency graph to determine the final XIG execution schedule. It is easy to see that the worst-case time complexity of MERGEXIG (or, the entire XIG optimization procedure) is $O(n^3|\mathcal{S}|\log n)$.

Next, we consider how to merge a pair of queries, namely, given a query pair (Q_1, Q_2), how to generate a single query Q to compute both Q_1 and Q_2. For a pair of queries that are not dependent on each other, the merged query can be simply expressed as:

<result> <q1>{Q_1}</q1> <q2>{Q_2}</q2> </result>

It is straightforward to separate and extract the results of Q_1 and Q_2 from the result of the merged query.

Now, consider a pair (Q_1, Q_2) where Q_2 uses the result of Q_1. In particular, consider a production $A \rightarrow \alpha$, and we want to merge the queries for computing $Inh(\mathtt{A})$ (Q_1) and $Inh(\mathtt{B})$ (Q_2), where B is in α. If Q_1 yields a sequence of values of $Inh(\mathtt{A})$, we want the merged query Q to compute a corresponding sequence of $Inh(\mathtt{B})$ values. We associate a "key" with each value of $Inh(\mathtt{B})$ in order to determine the position of the B element in the target XML document. The key of an $Inh(\mathtt{B})$ value is generated by concatenating the key of the corresponding $Inh(\mathtt{A})$ value \$x and an id f_{sk}(\$x). Here f_{sk} is a Skolem function that, given a value, generates a unique id (see, e.g. [Kos96] for discussions on Skolem functions). Using the keys, the synthesized attribute $Syn(\mathtt{A})$ can be computed by sort-merging the values of $Syn(\mathtt{B})$ for all B in α *w.r.t.* key values.

For example, recall the rules associated with a production $A \rightarrow B_1, \ldots, B_n$ (similarly for other productions). Let query Q_1 compute $Inh(\mathtt{A})$ and return either a single s-element

<s> <val> v </val> <key> k </key> </s>,

or a sequence of s-elements enclosed by a tag <seq>, where v is a value of $Inh(\mathtt{A})$ and k is the key of v. Then, the merged query for computing $Inh(\mathtt{B_i})$ is (abusing XQuery syntax):

let \$a := Q_1 **return**
{**if** \$a/s
then <s> <val>{Q_i(\$a/s/val)}</val>
<key>{(\$a/s/key, f_{sk}(\$a/s/val))}</key> </s>
else <seq> **for** \$a′ **in** \$a/seq/s
let \$v := \$a′/val
let \$k := \$a′/key
return <s> <val>{Q_i(\$v)}</val>
<key>{(\$k, f_{sk}(\$v))}</key> </s>
</seq>}

The query returns either a single pair ($Inh(\mathtt{B})$, key) or a sequence of such pairs depending on the input $Inh(\mathtt{A})$. (Note that the sibling and parent/child relations are captured by the keys.) This example shows how to merge a pair of queries with dependency on them.

It is worth mentioning that the query-merging strategy given above does not introduce any null values, in contrast to the out-union/outer-join approaches of [BCF+02, BCF+03, FMS01, CFI+00].

6.5 Experimental Evaluation

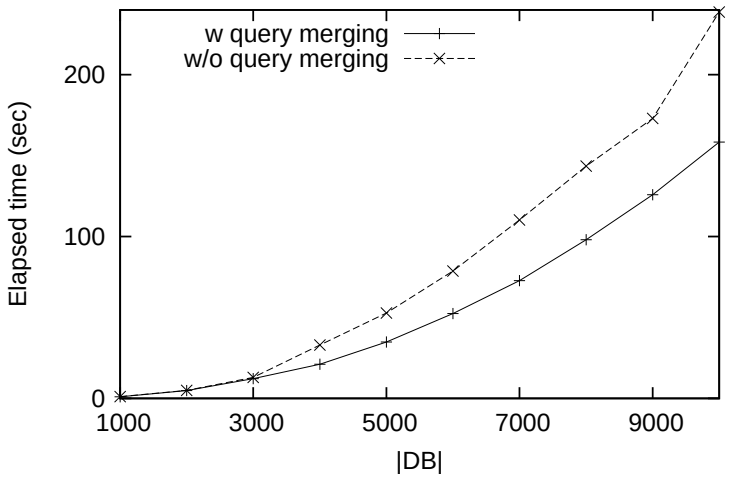


Figure 6.9: Effectiveness of query merging on XIG G_{dealer}

Next, the preliminary results from an experimental evaluation of the XIG-based techniques is presented. A prototype of XIG-based middleware has been built on top of the Galax XQuery engine (`db.bell-labs.com/galax`) and Java RMI. The source databases are built based on the source DTD D^S_{dealer} and D^S_{dealer} by using the Toxgene data generator (`www.cs.toronto.edu/tox/toxgene`). The database size, $|DB|$, is given as the number of cars. A fraction f of the cars are on sale. For the recursive definition of `feature` in the sale data (recall D^S_{sale} from Fig. 6.1), 1 to 3 random features are generated for each car and the depth of the recursion is limited to 2. The experiments were run on a distributed system connected by a local area Ethernet. Each site has a 2.4GHz Pentium 4 processor and 512M RAM. Unless otherwise stated, each experiment was run 5 times and the average is reported.

Query Merging. Figure 6.9 shows the impact of query merging on the performance of

the XIG G_{dealer} for different database sizes. Since G_{dealer} only involves a single server, scheduling is not needed here. The results clearly indicate that the evaluation strategy with query merging outperforms the one without merging. The performance gain is about 30% for large databases. Note that the gain comes from reducing the number of Galax calls, as Galax does not support query optimization and thus merged queries are not optimized by Galax. The performance gain from query merging is expected to be further improved pending the availability of optimization in XQuery engines (to our knowledge, no stable XQuery engine supports all of our queries and optimizations).

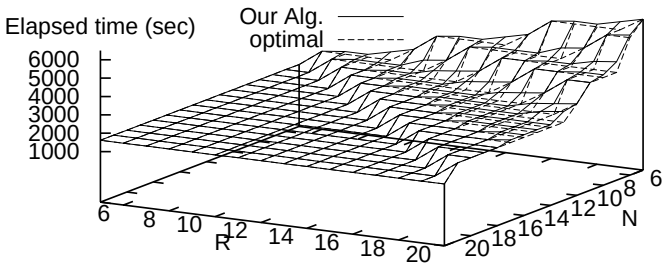


Figure 6.10: Scalability and benefits of query composability

Query Composability. The next set of experiments verifies the scalability and benefits of our XIG evaluation algorithm (namely, SCHEDXIG and MERGEXIG put together) with two workloads W_1 and W_2. To better demonstrate the impact of remote XIG calls, W_1 slightly extends the XIG $G(R,X)$ of Fig. 6.5 by adding a remote XIG which encodes the join in the rule for computing *Inh*(`car`), while W_2 further extends G_{dealer} in W_1 by adding an extra join on the car model. Both workloads were run on the distributed system. Figure 6.10 compares the evaluation time of W_2 obtained by using the evaluation algorithm with that of an optimal scheduling and merging strategy, which is computed manually as the XIGs involved are simple. In Fig. 6.10, $|DB|$ and f are fixed as 5000 and 10%, respectively. The number of servers N and the number of URIs R are varied from 5 to 20. The remote calls are uniformly distributed over the servers. The results show that our algorithm performs well; indeed, its performance nearly matches the optimal one. Furthermore, Fig. 6.10 indicates

that our algorithm also scales well – its evaluation time decreases when the number N of servers increases, i.e. it is roughly linear in $1/N$; moreover, the performance is better when the N/R ratio gets larger. The results of evaluating W_1 are similar.

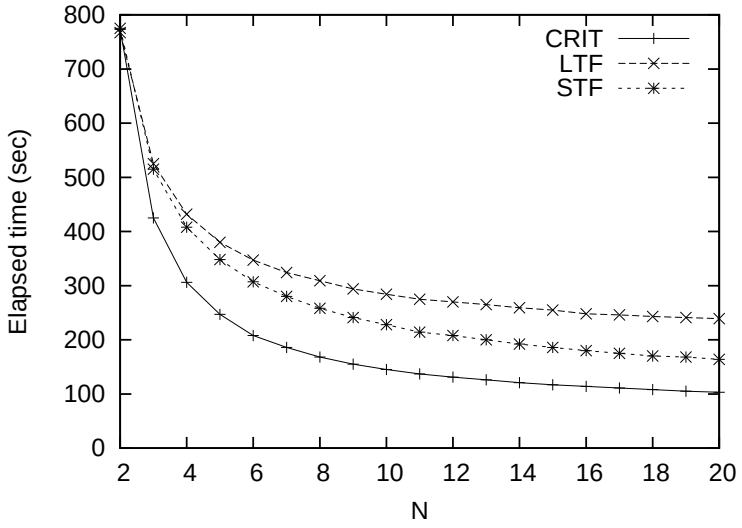


Figure 6.11: Effectiveness of XIG-Scheduling

Scheduling. To study workload sensitivity of our criticality-based XIG-*Scheduling* algorithm (denoted as *CRIT*), we compare its performance with two traditional scheduling algorithms *Shortest Task First (STF)* and *Longest Task First (LTF)* using randomly-generated XIG query-dependency graphs. Table 6.1 gives parameter settings for our random dependency-graph generator. Each node in a graph has a single parent (i.e. fan-in of 1), whereas node fan-out is chosen uniformly between 2 and 4. The length of root-to-leaf path is chosen uniformly between 4 and 8. The probability of a node being an XIG call is 0.5, and its execution site is distributed uniformly among all servers. The ranges of costs for queries and XIG-calls are determined based on the response times obtained by using our prototype. Figure 6.11 depicts the performance of the algorithms. Each simulation was run 100 times to obtain sufficient confidence intervals of average elapsed times. The number of servers, N, varies from 2 to 15. Clearly, when N is small (e.g. $N = 2$), scheduling is a non-issue and all algorithms perform similarly. However, as N increases, *CRIT* does better at exploiting parallelism, and it outperforms *STF* and *LTF* by more than 40% and 60%, respectively.

Parameter	Meaning	Value
PathLen	Length of root-to-leaf path	[4, 8]
NoRoots	No. of root nodes	[1, 5]
ProbXIG	Probability of XIG-call nodes	0.5
FanIn	Node fan-in	1
FanOut	Node fan-out	[2, 4]
QueryCost	Local query cost (msec)	[10, 300]
XIGCost	Remote XIG cost (msec)	[100, 3000]
N	No. of servers	[2, 15]

Table 6.1: Settings for dependency graph generation

These results show that our query-merging algorithm is effective for optimizing XIG evaluation, and that the XIG-scheduling technique significantly outperforms traditional scheduling algorithms.

6.6 Related Work

Data integration is the problem of combining data from distributed, heterogeneous sources to provide users with a unified interface. Without a data integration system, users have to remember the location of each data source, pose queries over these sources in different query languages and combine the results manually. A data integration system dramatically reduces this work and thus is desired in many applications. Traditionally, the unified interface in data integration is often defined as a global relational view. Recently, the role taken by relational views in data integration has been increasingly shifted to XML views. Several factors have contributed to this shift: First, the tree-structured XML data model can naturally represent broader range of data than the tabular-structured relational model. Second, with the fast development of the web and web services, huge amount of data is represented natively in XML format. Third, more and more tools are available to convert data in other formats to XML formats as demonstrated in the last chapter. Last but not least, XML has become a standard for data exchange and a large part of integrated data

often needs to be exchanged. Thus, XML data integration is highly demanded in modern information systems.

Although a number of integration systems have been developed for semistructured data and XML [BGL+00, BGK+02, CDSS98, GMPQ+97, CFI+00, FMS01, MZ98, PVM+02], they typically provide very little support for modularity or ensuring DTD-conformance, especially when the prescribed DTD is recursive and/or non-deterministic. Clio [PVM+02] derives schema and data mappings from constraints; it is unclear how it can ensure DTD conformance automatically. MIX [BGL+00] considers DTD checking/inference for XML integration, but the inference process is expensive, and does not provide any guidance for how to define a mapping that type-checks [PV00]. XML publishing systems such as SilkRoute [FMS01], XPERANTO [CFI+00, SSB+01b] and ROLEX [BGK+02] consider only a single relational source and do not take DTDs into account. Earlier systems [CDSS98, GMPQ+97, MZ98] are either developed for semistructured data without a type system, or based on schema-matching; it is unclear how they can automatically guarantee DTD-conformance when the source and target schemas involved are dramatically different, or if the integration depends on the *application* rather than merely upon the schemas. Furthermore, none of these systems addresses modularity for integration specifications. Similarly, in the realm of commercially-available systems, support for modular, DTD-directed XML data integration is either non-existent or still at a fairly primitive stage. Nimble's Integration suite (`www.nimble.com`) allows users to pose queries over distributed XML data sources to synthesize a result XML document but does not address the issues of schema conformance or modular integration specifications. BEA's WebLogic Integration and Liquid Data suites (`www.bea.com`) allow for XML-to-XML transformations through a visual mapping tool that allows users to specify simple matchings between schema elements; it is unclear how these tools can be used to specify complex, hierarchical integration with a complicated target DTD.

Active XML (AXML) [ABC+03a, MAA+03] proposes a novel notion of intentional XML documents with embedded function calls to remote Web services. AXML is designed to support data exchange and Web-service calls via an unlimited class of embedded functions; furthermore, it also supports XML data integration through the use of XML tree templates with embedded function calls. However, this template-based approach to integration can typically only produce mild variations of a fixed document structure. The functionality of

AXML for supporting embedded Web services is, in a sense, complementary to the problem of DTD-directed XML integration, where the goal is to construct an integrated view guaranteed to conform to a predefined, possibly complex DTD.

It is worth mentioning that XIGs are not targeted for providing the functionalities of AXML to support Web services; they are complementary to AXML by providing guarantee for generating XML documents that conform to predefined DTDs when it comes to XML integration, instead of producing mild variations of a fixed document.

Closest to this work are Attribute Integration Grammars (AIGs), a grammar-based formalism for schema-directed integration of relational data in XML [BCF$^+$02, BCF$^+$03]. AIGs extend a target DTD with tuple-valued attributes and SQL queries over the relations. These earlier proposals are, however, inadequate for XML integration. First, they are restricted to *flat, relational sources* [BCF$^+$02, BCF$^+$03]. Second, and perhaps most importantly, while AIGs guarantee schema-conformance, they are *not composable*: a large integration task must be specified with a *single* AIG on top of a large DTD. Developing an effective, modular solution for large-scale, DTD-directed XML data integration poses a whole new set of difficult research challenges, including the need for a significantly more powerful, composable formalism and novel optimization/evaluation techniques.

Chapter 7

Selective Exposure of the Integrated Data

In many applications users are allowed to access an XML document only by querying a view of the data. The need for this is evident in, for example, enforcing access control on XML data [CAYLS02, DdVPS00, FCG04]. To prevent improper disclosure of sensitive or confidential information of XML data residing in a server, the administrator defines an XML view for each group of users, consisting of all and only the information that the users are authorized to access. While the users may query the view, they are not allowed to directly query or access the underlying document (referred to as the *source*). With this comes the need to answer queries posed on the views. One way to do this is to first materialize the views and then directly evaluate queries on the views. However, it is often too costly to materialize and maintain a large number of views, a common scenario when many groups of users with different access privileges query the same source. A more realistic approach is to *rewrite* (aka. translate, reformulate) queries on the views into equivalent queries on the source, evaluate the rewritten queries on the source *without materializing the views*, and return the answers to the users.

This chapter studies how to rewrite XML queries posed on virtual XML views into equivalent queries on the underlying XML document. For XML queries we start with a fragment of XPath, which supports recursion (the descendant-or-self axis '//'), union and complex filters (predicates). This class of XPath queries is commonly used in practice and is essential to XQuery, XSLT and XML Schema. We consider XML views defined by annotating a

view DTD with a collection of (regular) XPath expressions, along the same lines as how commercial systems specify XML views [IBM, Ora, Mic05]. An XML view defined as above is a mapping $\sigma : D \rightarrow D_V$ in the global-as-view style, from XML documents of the *document* DTD D to documents of the *view* DTD D_V. When the view schema D_V is *recursively defined*, i.e. if some element type in D_V is defined in terms of itself, so is the view. The central technical problem studied in this chapter is:

The *rewriting problem* is to find an algorithm that, given a view definition σ and an XPath query Q over the view DTD D_V, computes an XPath query Q' over the document DTD D such that for any XML tree T of D, $Q(\sigma(T)) = Q'(T)$.

While there has been a host of work on rewriting XPath queries into SQL queries for XML views of relational data (see [KCKN04] for a survey), little previous work has considered rewriting XPath queries into XPath queries for XML views which can hide arbitrary nodes of XML data. In this context, query rewriting has only been studied for non-recursive XML views, over which XPath rewriting is always possible [FCG04]. However, query rewriting for *recursive* views is still an *open* problem [KCKN04].

Recursive DTDs naturally arise when, e.g., specifying biomedical data (see the Gene Ontology database, GO [EBI]); in fact [Cho02] shows that out of 60 real-world DTDs analyzed, more than half (35) of them were recursive. It is the reason that Oracle supports fully recursively defined XML views (AXSD [Ora]) and that IBM also allows a class of recursively defined XML view (DAD [IBM]). However desirable, the rewriting problem is more intriguing for recursively defined views, due to the interaction between recursion in XPath queries (e.g., '//') and recursion in the view definition.

Example 7.1: Consider a *hospital* DTD D shown as a graph in Fig. 7.1. A *hospital* document of D consists of a list of *department*s, and each *department* has a list of in-*patient*s (i.e. patients who are currently residing in the hospital; we use '$*$' on an edge to indicate a list). For each *patient*, the hospital maintains her name (*pname*), *address*, records of *visit*s, each including the visit *date* and *treatment* which is either a *test* or some *medication* (dashed edges indicate disjunction), as well as information about the treating *doctor*. Each *name*, *pname*, *street*, *city*, *zip*, *date*, *type*, *dname*, *specialty* has a single text node (PCDATA) as its child (omitted in the figure). The hospital also maintains family medical history by means of the recursively defined *parent* and *sibling*. It records the same information of ancestors

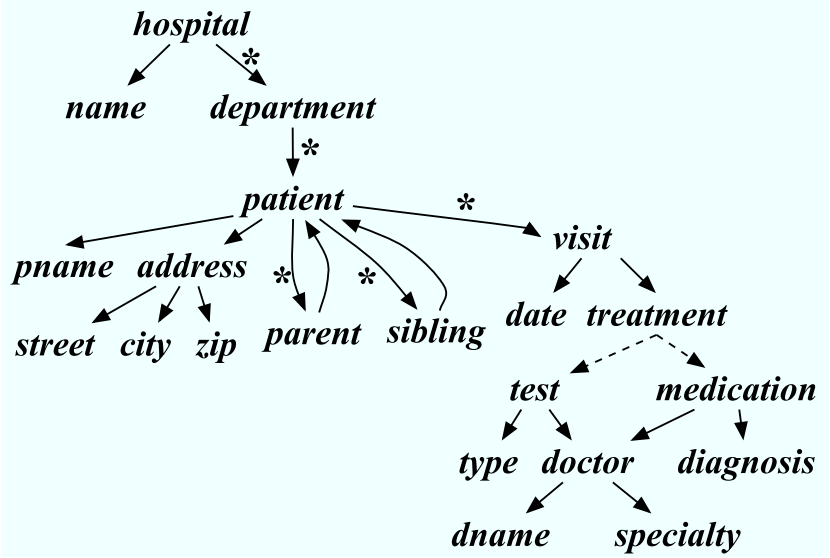
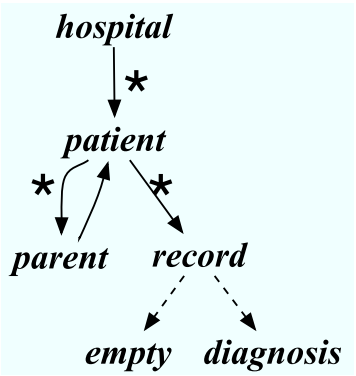


Figure 7.1: Example: document DTD D.



(a) view DTD D_V

production: *hospital* → *patient**
σ_0(*hospital,patient*) = *department/patient[visit/treatment/medication/diagnosis/text() = 'heart disease']* /*Q_1*/

production: *patient* → *parent**, *record**
σ_0(*patient, parent*) = *parent* /*Q_2*/
σ_0(*patient, record*) = *visit* /*Q_3*/

production: *parent* → *patient*
σ_0(*parent, patient*) = *patient* /*Q_4*/

production: *record* → *empty* + *diagnosis*
σ_0(*record, empty*) = *treatment/test* /*Q_5*/
σ_0(*record, diagnosis*) = *treatment/medication/diagnosis* /*Q_6*/

(b) view specification

Figure 7.2: Example: view DTD and view specification.

with those of in-patients, by sharing the description for *patient*s.

A view σ_0 is defined for a research institute studying inherited patterns of heart disease, with the *view* DTD depicted in Fig. 7.2 (the view is defined in Example 7.3). Obliged by the Patient Privacy Act, the view reveals only those *patient*s who have heart disease, along

with their *parent* hierarchy. While the institute may access *diagnosis* information of those patients and their ancestors, it is denied access to their *name*, *address*, *test* and *doctor* data.

Consider an XPath query Q posed on the view, which is to find patients whose ancestors also had heart disease:

$$Q: \quad patient[*//record/diagnosis/text()=\text{'heart disease'}].$$

Here $*$ denotes a wildcard, i.e., any element. However, it is impossible to rewrite Q on the view to an equivalent query (in the XPath fragment mentioned above) on the underlying *hospital* document. This is because '//' in Q is supposed to traverse only the *parent* hierarchy on the view, i.e., a sequence of the *(parent/patient)* pattern; however, when translated to a query Q' on the source, Q' necessarily retains '//' since the view DTD is recursive, and '//' in Q' may access *siblings* of those patients, although *siblings* are not in the view and are not allowed to be accessed. An incorrect translation may lead to serious security breach. □

In response to this both fundamental results and practical techniques for the rewriting problem have been developed in this chapter.

7.1 XML Security Sub-framework

Views are commonly used in traditional (relational) databases to enforce access control, and therefore provide a promising method to access XML data securely. In CLINSE, an XML security sub-framework has been designed to protect the integrated XML data. The sub-framework is based on the novel concept of *security views* proposed in [FCG04], which provide for each user group a virtual XML view consisting of all and only the information that the users are authorized to access, and a view DTD that the XML view conforms to.

As depicted in Fig. 7.3, the sub-framework consists of three primary modules (*view derivation* and *query rewriting*, *evaluation*) and four secondary modules (*access policy editor*, *security view editor*, *query editor*, and *result viewer*). Briefly, the secondary modules implement a user-friendly interface through which the user interacts with the system. The primary modules implement all the basic algorithms and functionality of the sub-framework. They are internal and thus users do not directly interact with them.

Central to the sub-framework is a number of *security views* which tailor the XML docu-

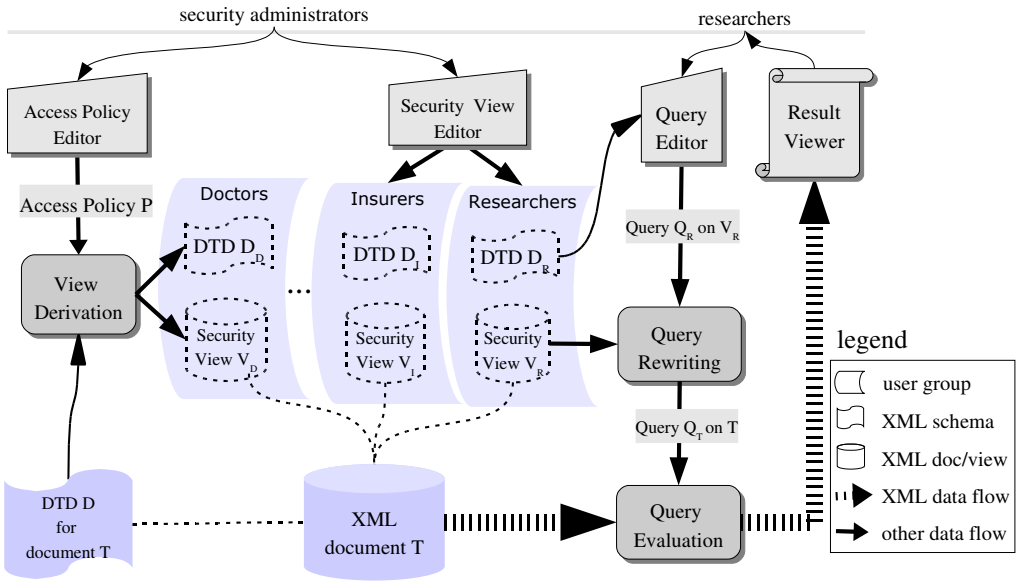


Figure 7.3: The XML security sub-framework

ment for different user groups by hiding the un-authorized information. Two types of users interact with the sub-framework, namely, *security administrators* who specify the access policies or security views for each user group, and *users in a certain group* who query the XML views to which they have been granted access.

To illustrate the sub-framework, suppose that several user groups, such as researchers, insurers and doctors, need to access the medical records in Fig. 7.1. As shown in Fig. 7.3, it works as follows. First, using the *access policy editor*, the security administrators specify the access policies P for each group as annotations in the DTD of the XML documents. The policies P are then passed to the *view derivation module* where a set of security view definitions V_R, V_I, V_D and their DTDs D_R, D_I, D_D are automatically derived from P for the groups of researchers, insurers, and doctors, respectively. Next, users in each group are allowed to pose queries over the virtual security view using the *query editor*. This process is assisted by providing users with a corresponding view DTD. For instance, a user U_R in the group of researchers poses a query Q_R over view V_R. In the *query rewriting module*, this query Q_R is subsequently rewritten into a new query Q_T over the underlying document T. Query Q_T is passed to the *query evaluation module* to be executed over the document T. Finally, the result of Q_T (and therefore Q_R) is shown in the *result viewer* to the user U_R. In the environments requiring more flexibilities, the views V_R, V_I and V_D could also

be manually defined by the security administrators with the assistance of the *security view editor*.

In the worst case, four languages are involved in the sub-framework: the *access specification language* L_A and the *view specification language* L_V are used by the security administrators to specify access policies and security views, respectively; the *view query language* L_Q^V and the *document query language* L_Q^T are used by the users to pose queries over the XML data. L_V and L_Q^T are also used by the view derivation and query rewriting modules, respectively, for representing the automatically generated view definitions and queries. Solutions for the view derivation have been provided in [FCG04]. Moreover, in the settings where the security views are manually specified, view derivation module is not needed. In the remainder of this chapter, the query rewriting and evaluation problems, which are not fully solved in [FCG04], are investigated and the requirements of languages L_V, L_Q^V and L_Q^T are studied.

7.2 XML Queries and View Specifications

In this section we review the candidates of view specification language L_V, view query language L_Q^V and document query language L_Q^T considered in this chapter.

7.2.1 XPath and Regular XPath

In this chapter, the downward fragments of XPath and regular XPath, i.e., $\mathcal{X}^{\downarrow,*;*}_{\cup;[\neg,=]}$ and $\mathcal{X}^{\downarrow;*}_{\cup,*;[\neg,=]}$ defined in Section 5.3, are considered. Hereafter they will be simply written as $\mathcal{X}$ and $\mathcal{X}_R$, and the simplified syntax is adopted. For example, regular XPath [Mar04b] $\mathcal{X}_R$ is simplified as:

$$Q ::= \varepsilon \mid A \mid \downarrow \mid Q/Q \mid Q \cup Q \mid Q^* \mid Q[q],$$
$$q ::= Q \mid Q/text() = \text{`}c\text{'} \mid \neg Q \mid Q \wedge Q \mid Q \vee Q$$

where ε is the empty path (*self*), A is a label (tag), $\downarrow$ is a wildcard (i.e., the $*$ inside of a node test in the un-simplified syntax), '$\cup$' represents *union*, '$/$' is the *child-axis*, and $*$ is the Kleene star; $[q]$ is referred to as a *filter*, in which Q is an $\mathcal{X}_R$ expressions, c is a string constant, and $\neg, \wedge, \vee$ are the Boolean negation, conjunction and disjunction, respectively.

Note that, instead of the $*$ used in Section 5.3, $\downarrow$ is used to denote a wildcard to avoid the confusion with a Kleene star.

Like XPath queries, when an $\mathcal{X}_R$ query Q is evaluated at a node v in an XML tree T, it returns the set of nodes of T reachable via Q from v, denoted by $v[\![Q]\!]$.

Similarly, the simplified syntax of downward XPath $\mathcal{X}$ is defined by replacing Q^* with '//' in the definition above.

Example 7.2: Consider an XML document T conforming to the document DTD D in Fig. 7.1. The regular XPath query

$$Q = \textit{department/patient}[\, q_0 \wedge (q_1/(q_1)^*)]/\textit{pname}$$
$$q_0 = \textit{visit/treatment/medication/diagnosis/text()} = \text{“}\textit{heart disease}\text{”}$$
$$q_1 = \textit{parent/patient}[\neg q_0]/\textit{parent/patient}[q_0]$$

when evaluated on T, returns the names of patients who have heart disease and the disease appears in their ancestors but always skips a generation. Such queries, which look for certain patterns, are often encountered in medical research. Note that the query is in the fragment $\mathcal{X}_R$, but is not expressible in the XPath fragment $\mathcal{X}$. □

Regular XPath extends regular expressions by allowing filters [Mar04b, Koz97], and extends XPath by supporting general Kleene closure Q^* as opposed to restricted recursion '//'. The tradeoff of the expressive power is the additional complexity for query evaluation: (a) recursion can no longer be captured by a simple ancestor-descendant labeling as for its XPath counterpart [LM01, KMS02, SHYY05]; and (b) worse still, recursion in an $\mathcal{X}_R$ query may be nested: the sub-query Q of Q^* may itself contain Kleene closure, which we do not encounter when evaluating XPath queries.

This chapter focuses on regular XPath queries with only downward modalities since they are most commonly used in practice. As will be seen shortly, rewriting queries is already challenging in this setting. It is thus necessary to understand rewriting of these basic queries before dealing with full-fledged XPath or XQuery.

7.2.2 XML Views

We consider views defined by annotating a DTD [FCG04]. This is similar in spirit to XML view specification in commercial systems, e.g. annotated XSD's (AXSD) in Oracle

XML DB [Ora] and Microsoft SQL Server 2000 SQLXML [Mic05], and Document Access Definitions (DAD) of IBM DB2 XML Extender [IBM].

Specifically, an XML view is a mapping $\sigma : D \rightarrow D_V$, where D is a *document* DTD, D_V is a *view* DTD. Given an XML document T of D, the mapping generates an XML view $\sigma(T)$ that conforms to the view DTD D_V. More specifically, for each element type A and its child type B in D_V (i.e., each edge (A,B) in the DTD graph of D_V), σ maps (A,B) to a query $\sigma(A,B)$ defined on documents T of D. Intuitively, given an A element, $\sigma(A,B)$ generates its B children in the view by extracting data from T. The query $\sigma(A,B)$ is in the regular XPath fragment $\mathcal{X}_R$ given above. The XML view is *recursive* if the view DTD D_V is recursive.

Example 7.3: The view σ_0 described in Example 7.1 can be defined based on the view DTD D_V of Fig. 7.2(a), as shown in Fig. 7.2(b). □

To give the semantics of σ, we present a materialization strategy that, given an XML tree T of the document DTD D, computes the view $\sigma(T)$, as follows. A partial tree T_V is initialized by copying the root of T and treating it as the root of T_V, and this node is marked *unexpanded*. The tree T_V is then grown by repeatedly selecting an unexpanded b (of some element type A), evaluating the query $\sigma(A,B)$ for each child type B of A to generate the children of b, and marking b *expanded*. Specifically, we find the production $p = A \rightarrow P(A)$ in D_V, and generate the children of b based on the structure of $P(A)$ as follows.

(1) If $P(A)$ is $B_1, \ldots, B_n$, then for each B_i, the query $\sigma(A,B_i)$ is evaluated on the document T at the context node b. If B_i is of the form B^*, then each node returned by the query is treated as a distinct B child of b in the partial tree T_V. If B_i is of the form B and the query returns a single node, the node is treated as a B child of b in T_V. Otherwise the computation aborts for violating the production $A \rightarrow P(A)$ of the view DTD. In both cases, if the view DTD enforces a different label to the nodes returned by the mapping query, these nodes will be re-labeled to B_i in the view.

(2) If $P(A)$ is $B_1 + \cdots + B_n$, then for each $i \in [1,n]$, the query $\sigma(A,B_i)$ is evaluated on T at context node b. If there exists one and only one $i \in [1,n]$ such that $\sigma(A,B_i)$ returns a nonempty set of nodes without violating the cardinality constraint of B_i as described in (1) above, then these nodes are treated as the children of b in T_V; otherwise, the computation aborts. The returned nodes will be re-labeled similarly when there are conflicts between

the labels in the view and in the document.

(3) If $P(A)$ is *str*, the query $\sigma(A, str)$ is evaluated on T at context node b. If it returns a single text node in T, and the node is treated as the only child of b in T_V; otherwise, the computation aborts.

(4) If $P(A)$ is ε, nothing needs to be done.

The *element* children of the node b become new unexpanded and are also processed. The process proceeds until the partial tree T_V cannot be further expanded, i.e., it has no unexpanded node, or the computation is aborted. The fully expanded T_V is the view $\sigma(T)$. Note that $\sigma(T)$ is guaranteed to *conform to the view* DTD D_V.

Under this view specification language, there is a many-to-one correspondence between the nodes in the view and the nodes in the underlying XML document: no new XML node is constructed in the view; each XML node in the view is mapped from the XML document through a regular XPath query. We say a node in the view σ and a node in the XML document are *identical under view* σ if they are corresponded to each other in the definition of σ.

Now we are able to define the query rewriting problem more precisely:

The *rewriting problem* is to find an algorithm that, given a view definition σ and a query Q over the view DTD D_V, computes a query Q' over the document DTD D such that for any XML tree T of D, the answer nodes of $Q(\sigma(T))$ and those of $Q'(T)$ are identical under view σ.

In W3C XPath specification, the answer of a query is node set, number, string or boolean. In our extended XPath fragment, both the original query on the view and the rewritten query on the XML document return a node set(number, string or boolean answer does not apply to this fragment). The two node sets are identical under the view definition. If the user requires a node set as the answer, this is sufficient. In the cases where the user also requires the subtrees rooted at each node in the returned node set, more processing are needed.

The above defined view has a property: a subtree of the view, referred to as *subview*, could be evaluated without materializing other parts of the view. To materialize a subview, a context node in the XML document needs to be mapped as the root of the subview. This provides the flexibility to materialize arbitrary subviews to save unnecessary computations.

In the query rewriting scenario where the user requires subtrees as the answer, the answering subtrees could be obtained by materializing the subviews rooted at the returned nodes of the rewritten query. Note that the materialization of these subviews can not be avoided in any query answering mechanism, based on either virtual or materialized views, because the subviews themselves are parts of the answers.

Example 7.4: Given a *hospital* document T, σ_0 generates a view $\sigma_0(T)$ top-down, which conforms to the view DTD of Fig. 7.2(a). The query Q_1 (i.e., $\sigma_0(\textit{hospital}, \textit{patient})$) extracts from T those *patient*s who have heart disease. For the patients extracted by Q_1, (a) Q_2 finds their *parent* nodes, which are in turn processed by Q_4 and then inductively by Q_2 and Q_3 to form the *parent* hierarchy, and (b) Q_3 finds the *record* (i.e., *visit*) data, which can be either be *empty* (i.e., *test*) or *diagnosis*, handled by Q_5, Q_6, respectively. Note that if *test* node is returned, it is re-labeled to *empty* in the above step.

Observe the following. (a) While *patient* is recursively defined, the process terminates when Q_2 at *patient* nodes returns an empty set, i.e., when the *parent* records of those *patient*s are not available in T. (b) The choice of *empty* or *diagnosis* under a *record* is determined by the results of the queries Q_5 and Q_6 at the *record*. That is, recursion and disjunction are handled following a data-driven semantics. (c) The XPath query $\sigma_0(A, B_i)$ is evaluated at an A element in T, i.e., $\sigma_0(A, B_i)$ is defined relative to A elements. □

7.3 The Closure Property of (Regular) XPath

We next establish results for the closure property of XPath and regular XPath query rewriting. Formally, an XML query language L is *closed under rewriting* if there exists a function $F : L \to L$ that, given any view definition $\sigma : D \to D_V$ and any query Q in L over D_V, computes query $Q' = F(Q)$ in L such that for any document T of D, $Q(\sigma(T)) = Q'(T)$. While one may consider translating Q to an equivalent Q' in a richer language, e.g. XQuery or XSLT, it is vastly preferable to have an XPath translation since it is more efficient to evaluate and optimize XPath queries than queries in the aforementioned Turing-complete languages. In other words, the closure property is desirable since rewriting should not be penalized by paying the higher price for evaluating and optimizing queries in a richer language than that of the original query.

It was shown in [FCG04] that the class $\mathcal{X}$ of XPath queries defined in Section 7.2 is closed under query rewriting for *non-recursive* views. However, it is shown below that in the presence of recursion in a view definition, this is no longer the case (even when the annotating queries are in $\mathcal{X}$).

Theorem 7.3.1 *For recursively defined* XML *views, the fragment $\mathcal{X}$ is not closed under query rewriting.*

Intuitively, the complication is introduced by '//' in $\mathcal{X}$ queries posed on a recursive view. It is impossible to rewrite '//' by enumerating the matching label paths in the view DTD, since it may lead to infinitely many paths due to the recursion in the view DTD. Thus '//' needs to be captured by a recursive operator over the document which is, often necessarily, the Kleene star operator. A key property of Kleene star, not shared by '//', is that it can prevent the traversal of data that are in the document but not in the view, which is of central importance in the security setting, among other things.

Proof:

Consider the query $Q_0 = (\downarrow / \downarrow)^*$. When it is evaluated at the root of an XML tree T, it retrieves all nodes in T which are an even number of steps away from the root. It is known that this query Q_0 is not first order definable on trees [Tho84], and thus not expressible in XPath [Mar04b]. We now construct an XML view σ_0 and an XPath query Q_1 on the view, such that *any* rewritten query Q_1' of Q_1 on the source document is equivalent to Q_0. Since query Q_0 is not expressible in XPath, the rewritten query Q_1' can not be in XPath, either. This shows that XPath is not closed under query rewriting.

It remains to construct view σ_0 and query Q_1. Since we do not want to impose any restrictions on document T, we set its DTD D to be empty. We define the XML view $\sigma_0 : D \rightarrow D_V$ recursively as:

production: $r \rightarrow A^*$
$\sigma_0(r,A) = \downarrow / \downarrow$

production: $A \rightarrow A^*$
$\sigma_0(A,A) = \downarrow / \downarrow$.

where A is an arbitrary label. Clearly $\sigma_0(T)$ extracts all nodes which are an even number of steps away from the root of T in the same way as query Q_0 does. By simply defining

$Q_1 = //A$, i.e., by retrieving all the nodes in $\sigma_0(T)$, it is clear that any rewritten query on the source document should be equivalent to Q_0. □

In contrast, the fragment $\mathcal{X}_R$ of regular XPath given in the last section is closed under query rewriting:

Theorem 7.3.2 *For arbitrary* XML *views (recursive or non-recursive), $\mathcal{X}_R$ is closed under rewriting.*

Proof: This is a direct consequence of the equivalence of MFA and $\mathcal{X}_R$ queries [FGJK07] and Theorem 7.5.1. □

Given that $\mathcal{X}_R$ subsumes $\mathcal{X}$, an immediate result of Theorem 7.3.2 is that all $\mathcal{X}$ and $\mathcal{X}_R$ queries on any view can be rewritten to equivalent $\mathcal{X}_R$ queries on the source. To perform the rewriting, we can traverse the view DTD graph D_V via Q, replacing each encountered edge (A,B) with $\sigma(A,B)$. A tricky issue concerns the translation of p^* (or '//') at a context node A, denoted by $\text{REG}_x(p^*,A)$. The rewritten $\mathcal{X}_R$ query $\text{REG}_x(p^*,A)$ is to capture all the label paths from A to nodes reached via p^*. This often requires to construct a NFA to characterize these paths. This NFA is then converted into a regular expression in order to obtain the expression for p^*.

Example 7.5: Recall the $\mathcal{X}$ query Q given in Example 7.1 and the view σ_0 defined in Example 7.3. While Q cannot be rewritten into Q' in $\mathcal{X}$ on the source T, it can be rewritten to an equivalent regular XPath query Q_r in $\mathcal{X}_R$ over T (Using the queries Q_1, Q_2, Q_3, Q_4 and Q_6 from the view specification in Fig. 7.2(b)):

Q_r : $Q_1[Q_2/Q_4/(Q_2/Q_4)^*/Q_3/Q_6/text()$='heart disease'],
i.e., *department/patient*[*visit/treatment/medication/diagnosis/*
text()='heart disease' ∧ *parent/patient/(parent/patient)**
visit/treatment/medication/diagnosis/text( )='heart disease'].

□

Although it is always possible to rewrite a (regular) XPath query on a view to an equivalent regular XPath query on the source, it is often prohibitively expensive if it is to directly compute $\mathcal{X}_R$ queries as output. Indeed, the rewriting problem subsumes the problem for translation from NFA's to regular expressions. The latter problem is EXPTIME-complete [EZ76]: the size of the explicit representation of a regular expression is exponential in the size of the NFA. Worse still, it remains exponential even if the NFA is acyclic.

Query rewriting	Views	Closure	Complexity
from $\mathcal{X}$ to $\mathcal{X}$	non-rec.	Yes [FCG04]	EXPTIME-complete
from $\mathcal{X}$ to $\mathcal{X}$	recursive	No	NA
from $\mathcal{X}$ to $\mathcal{X}_R$	arbitrary	Yes	EXPTIME-complete
from $\mathcal{X}_R$ to $\mathcal{X}_R$	arbitrary	Yes	EXPTIME-complete

Figure 7.4: Closure property and complexity

Indeed, [FGJK07] has shown that there exist a view definition $\sigma : D \rightarrow D_V$ and a query Q in $\mathcal{X}$ such that for any Q' in $\mathcal{X}_R$, if $Q(\sigma(T)) = Q'(T)$ for all XML trees T of D, then the size $|Q'|$ of Q', when represented as an $\mathcal{X}_R$ query, is exponential in $|Q|$ and the size $|D_V|$ of D_V. The lower bound remains intact even when D_V is non-recursive.

The main results of query rewriting are summarized in Fig. 7.4.

7.4 Mixed Finite State Automata

The possible exponential size of the rewritten queries tells us that a direct rewriting into (regular) XPath is beyond reach in practice. To overcome this, in this section a new representation of $\mathcal{X}_R$ queries, referred to as *mixed finite state automata* (MFA) is introduced. Along the same lines as NFA for regular expressions, MFA characterize $\mathcal{X}_R$ queries and avoid the exponential blowup of rewriting. Leveraging MFA we shall present a practical solution to the rewriting problem by providing (a) a low polynomial-time algorithm for rewriting $\mathcal{X}_R$ queries on a view into the MFA-presentation of equivalent $\mathcal{X}_R$ queries on the source (Section 7.5), and (b) a linear-time algorithm for directly evaluating the MFA-represented $\mathcal{X}_R$ queries on the source (Section 7.6).

While a regular expression can be efficiently represented as a graph or a NFA, for $\mathcal{X}_R$ queries a notion of automaton representation is not yet available. The difficulties of characterizing an $\mathcal{X}_R$ query Q as an automaton include the following: (a) Q typically involves both "selecting" paths that are to extract and return nodes, and filters that constrain the extraction; (b) a filter $[q]$ in Q may involve Boolean operators '$\wedge, \vee, \neg$' and constant test $p/text() = 'c'$, which are not encountered in regular expressions; (c) worse still, it may be nested: q itself may be a query of the form $p[q_1]$; and (d) the sub-query p of p^* may itself

contain Kleene closure.

Mixed finite state automata (MFA)**.** In light of this we define an MFA $\mathcal{M}$ as a *selecting automaton* (SA) in which a state may be annotated with a *filtering automaton* (FA). Intuitively, the SA in $\mathcal{M}$ is to capture the selecting paths of an $\mathcal{X}_R$ query Q and the FA's are to characterize the filters in Q.

Formally, an MFA $\mathcal{M}$ is defined to be $(\mathcal{N}, \vec{\mathcal{A}})$, where $\mathcal{N}$ and $\vec{\mathcal{A}}$ are defined as below:

(i) selecting automaton $\mathcal{N} = (K, \Sigma, \delta, s, F, \lambda)$ is a variation of *non-deterministic finite automaton* (NFA), where

K is the finite set of states;

Σ is the input alphabet, i.e. the set of labels in XML tree $\cup \{\varepsilon\}$ where ε is an empty string;

$\delta : K \times \Sigma \rightarrow 2^K$ is the transition function, where 2^K denotes the power set of K;

$s \in K$ is the start state;

$F \subseteq K$ is the set of final states; and

λ is a partial mapping from K to a set of names X_i, i.e., a state in $\mathcal{N}$ may be annotated with a single name X_i.

Note that, K, Σ, δ, s, F are the states, alphabet, transition function, start state and final states as in the standard NFA definition; λ does not appear in standard NFA definition.

(ii) $\vec{\mathcal{A}}$ is a set of bindings $X_i = \mathcal{A}_i$, where X_i is a name used in selecting automaton $\mathcal{N}$ to annotate a state, $\mathcal{A}_i$ is a filtering automaton. Filtering automaton $\mathcal{A} = (K, \Sigma, \delta, s, F)$ is a modified *alternating finite state automaton* (AFA) [Yu96], where

K is the finite set of states;

Σ is the input alphabet, i.e. the set of labels in XML tree $\cup \{\varepsilon\}$ where ε is an empty string;

$s \in K$ is the start state;

$\delta : K \times \Sigma \rightarrow 2^K$ is the transition function; and

$F \subseteq K$ is the set of final states optionally annotated with predicates of the form *text()='c'*.

Here the states K is partitioned into K_{op}, K_l and F, where K_{op} is a set of *operator states* marked with AND, OR or NOT, K_l is a set of *transition* states, and F is the final states.

The transition function δ is defined as follows.

(1) For a state s_1 in K_{op}, δ is only defined for empty string ε and $\delta(s_1,\varepsilon) = K'$, where K' is a subset of K. In particular, if s_1 is marked with NOT, K' has a single state in it.
(2) For each state s_2 in K_l, δ is only defined for a single label $A \in \Sigma$ and $\delta(s_2,A)$ contains a single state in K.
(3) δ is not defined for any state in F.

Observe that except for operator states marked with AND or OR, from each state at most one state can be reached via δ. These operator states capture Boolean operators $\wedge, \vee$ and $\neg$ in $\mathcal{X}_R$ filters.

The result of evaluating an MFA $\mathcal{M} = (\mathcal{N}, \vec{\mathcal{A}})$ at a node n in an XML tree T, i.e. $n[\![\mathcal{M}]\!]$, is the set of nodes in T that is associated with a final state of the selecting automaton $\mathcal{N}$ in a successful run. More specifically, the MFA $\mathcal{M}$ runs on tree T by associating a set of states in the selecting automaton and filtering automata to certain nodes in T as follows:
(a) First, MFA $\mathcal{M}$ initializes a set $cur = \{s\}$ as the current states for the selecting automata $\mathcal{N}$, transitively adds each state $s_2 \in \delta(s_1,\varepsilon)$ where $s_1 \in cur$ to cur and associates cur to the XML node n.
(b) For each state $s' \in cur$ that is annotated with a name X_s and there is a binding $X_s = \mathcal{A}_s$ in $\vec{\mathcal{A}}$ which binds the filtering automaton $\mathcal{A}_s = (K_s, \Sigma, \delta_s, s_s, F_s)$ to state s', MFA $\mathcal{M}$ begins to run $\mathcal{A}_s$ by initializing a set $cur_s = \{s_s\}$ as the current states for $\mathcal{A}_s$, transitively adding each state $s_2 \in \delta(s_1,\varepsilon)$ where $s_1 \in cur_s$ to cur_s and associating cur_s to node n.
(b.1) For each state $s' \in cur_s \cap K_l$, if a transition $s'' \in \delta(s',A_i)$ exists and A_i is the label of a child n_i of node n, $\mathcal{A}$ adds state s'' to the new current state set cur_{si} and associates node n_i with cur_{si}. $\mathcal{A}$ again transitively adds states reachable through ε transitions to cur_{si} and then repeats from step (b.1). A boolean value is assigned to each state of $\mathcal{A}$. A state $s' \in K_l$ is true if and only if its child state is true. If it has no child state, it is assigned false.
(b.2) For each state $s' \in cur_s \cap F$, if it is annotated with predicate *text()='c'*, assign the boolean result of evaluating this predicate at node n to s'. Otherwise, assign true to s'.
(b.3) For each state $s' \in cur_s \cap K_{op}$, the boolean value of s' is assigned as follows: when s' is marked with AND, s' is true if and only if s'' is true for *every* transition $s'' \in \delta(s',\varepsilon)$; when s' is marked with OR, s' is true if and only if a transition $s'' \in \delta(s',\varepsilon)$ exists such that s'' is true; when s' is marked with NOT, s' is true if and only if s'' is false for the transition $s'' \in \delta(s',\varepsilon)$.
(b.4) The filtering automaton $\mathcal{A}$ returns true if and only if its start state is assigned true.

(c) If no associated filtering automaton $\mathcal{A}_s$ returns false, MFA $\mathcal{M}$ continues to run the selecting automaton $\mathcal{N}$ at node n.
(c.1) For each child n_i of node n and each transition $s'' \in \delta(s', A_i)$ where $s' \in cur$, if A_i is the label of node n_i, $\mathcal{N}$ adds state s'' to the new current state set cur_i and associates node n_i with cur_i.
(c.2) If there is no child node (i.e. current node is a leaf) or the new current state set cur_i are all empty, MFA $\mathcal{M}$ stops. In this situation, if non of the final states of selecting automata $\mathcal{N}$ have been reached before, the run fails and MFA $\mathcal{M}$ returns an empty node set as the result. Otherwise, the run succeeds and MFA $\mathcal{M}$ returns all the XML nodes that is associated with some final states of $\mathcal{N}$.
(c.3) Otherwise, $\mathcal{N}$ continues to process each child node that is associated with non-empty state set cur_i. $\mathcal{N}$ again transitively adds states reachable through ε transitions to cur_i and then repeats from step (b).

Note that both the selecting automaton and the filtering automata are variations of word automata, but their semantics are modified such that they run on the tree. They are different from tree automaton. For example, in a top down unranked tree automaton, the transition function is usually defined as $\delta : K \times \Sigma \to 2^{K^*}$ such that $\delta(s, A_i)$ is a regular string language over K^* for every $A_i \in \Sigma$ and $s \in K$ [Nev02b] in contrast to $\delta : K \times \Sigma \to 2^K$ in our definition. In an alternating tree automaton, the transition function is usually defined as $\delta : K \times \Sigma \to B^+(N \times K)$ where $B^+(X)$ is a set of Boolean formulas over X such that $\delta(s, A_i) \in B^+(\{1, \ldots, k\} \times K)$ for each $A_i \in \Sigma$, $s \in K$ and k is the arity of the current tree node [Var97].

Example 7.6: Consider an $\mathcal{X}_R$ query Q_0 posed on an XML tree conforming to the DTD of Fig. 7.2(a), which is to find all patients who have an ancestor diagnosed with heart disease:

Q_0 = (*patient*/*parent*)*/*patient*[q_0],
q_0 = (*parent*/*patient*)*/*record*/*diagnosis*[*text()* ="heart disease"].

Consider MFA $\mathcal{M}_0$ in Fig. 7.5. It consists of a *selecting* automaton $\mathcal{N}$ (shown at the top of the figure), and a filtering automaton $\mathcal{A}_0$, corresponding to the filter q_0 (shown at the bottom). The MFA $\mathcal{M}_0$ is *equivalent* to Q_0, in the sense that when *evaluating* $\mathcal{M}_0$ at a node n in an XML tree T (described below), it returns the same set $n[\![\mathcal{M}_0]\!]$ of nodes as $n[\![Q_0]\!]$.

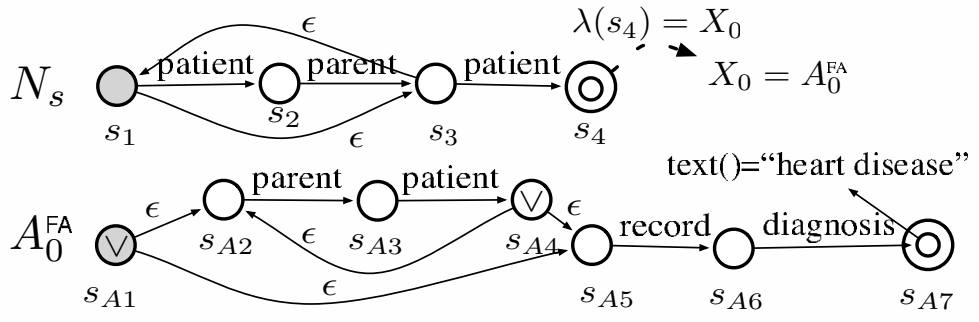


Figure 7.5: SA $\mathcal{N}$ and FA $\mathcal{A}_0$ in Example 7.6

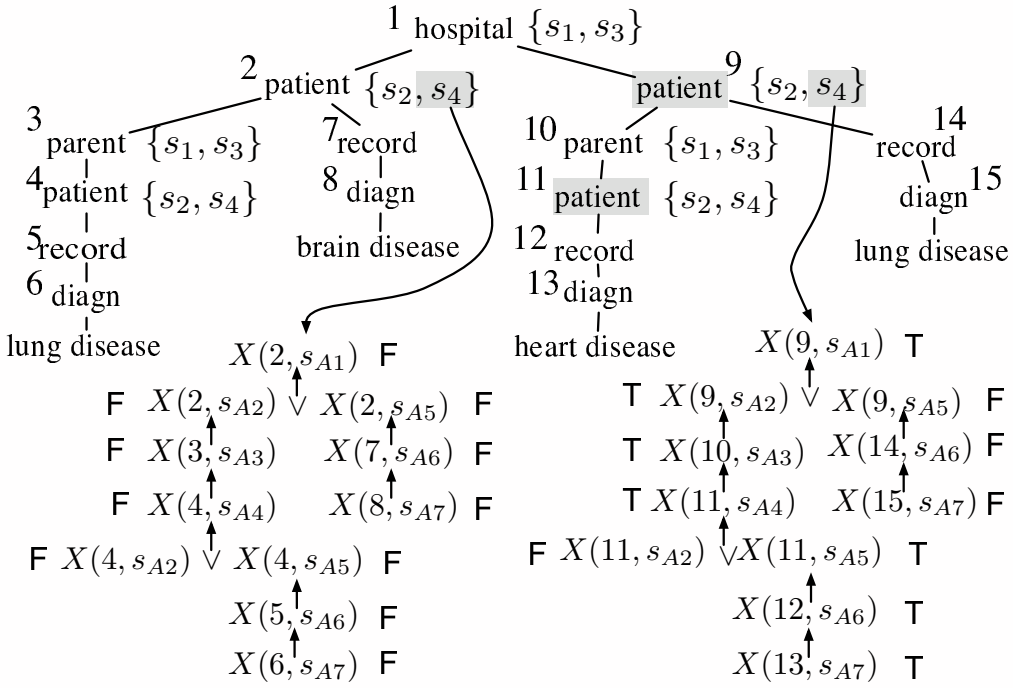


Figure 7.6: Conceptual evaluation of $\mathcal{M}_0$

The (conceptual) evaluation of $\mathcal{M}_0$ is illustrated, by example, in Fig. 7.6. At the root node 1 of the tree, $\mathcal{M}_0$ associates a set $\{s_1, s_3\}$ of $\mathcal{N}$ states, where s_1 is the start state of $\mathcal{N}$ and s_3 is reached from s_1 via an ε-transition. It then inspects the children of node 1: for all its children labeled *patient* (nodes 2 and 9), it associates them with states s_2, s_4, moves down to these children and processes them inductively, in parallel. At a node associated with state s_2, for all its children labeled *parent* (nodes 3 and 10) it associates them with

states s_1, s_3 and processes them in the same way as at the parent node of the tree. In the case of state s_4, since this state is annotated with $\mathcal{A}_0$, any node associated with state s_4 must also evaluate $\mathcal{A}_0$ (the evaluation of $\mathcal{A}_0$ is described below). This is the case for both nodes 2 and 9. Since s_4 is a final state, if $\mathcal{A}_0$ evaluates to true, the corresponding node is added to $n[\![\mathcal{M}_0]\!]$ (the *answer* of $\mathcal{M}_0$).

When the FA $\mathcal{A}_0$ is invoked, e.g., at node 2, a Boolean value $2[\![\mathcal{A}_0]\!]$ is computed as follows: $\mathcal{A}_0$ associates a Boolean variable $X(2, s_{A1})$ with node 2, whose value is to be computed and treated as $2[\![\mathcal{A}_0]\!]$, where s_{A1} is the start state of $\mathcal{A}_0$. It then traverses the subtree rooted at node 2 top-down. From s_{A1} there are two ε-transitions to s_{A2} and s_{A5}, and thus node 2 is also associated with variables $X(2, s_{A2})$ and $X(2, s_{A5})$ for these FA states. Since s_{A1} is an OR state, $X(2, s_{A1})$ is computed via $X(2, s_{A2}) \vee X(2, s_{A5})$. To compute $X(2, s_{A5})$, it inspects the children of node 2: if no child is labeled *record*, no $\mathcal{A}_0$ transition can be made from s_{A5} and $X(2, s_{A5})$ is assigned false; otherwise, for *all children* labeled *record*, in this case node 7, it associates a variable $X(7, s_{A6})$, moves down to these children and process them in parallel. Inductively, $X(7, s_{A6})$ is true if node 7 has a child labeled *diagnosis* and carrying text "heart disease", and if so, $X(2, s_{A5})$ is assigned true as well. Similarly, $X(2, s_{A2})$ is computed and becomes true if it has a descendant that is reachable via *(parent/patient)*/record/diagnosis* and carries text "heart disease". If either $X(2, s_{A2})$ or $X(2, s_{A5})$ is true, then $X(2, s_{A1})$ is true and so is the output $2[\![\mathcal{A}_0]\!]$. This is not the case here, however, and $\mathcal{A}_0$ returns false. □

Observe the following. (a) Although $\mathcal{A}_0$ traverses the subtree top-down, the Boolean variables are computed bottom-up. (b) In $\mathcal{A}_0$ the only operator states are OR states (s_{A_1}, s_{A4}); but AND and NOT states can be processed similarly. (c) The conceptual evaluation requires multiple passes over a subtree, one pass for each filter. In contrast, our evaluation algorithm in Section 7.6 requires only one pass of the input tree, regardless of the number of filters.

Equivalence of MFA and X_R queries. An MFA $\mathcal{M}$ and an X_R query Q are *equivalent* if for each XML tree T and any node n in T, $n[\![\mathcal{M}]\!] = n[\![Q]\!]$, where $n[\![\mathcal{M}]\!]$ (resp. $n[\![Q]\!]$) denotes the result of evaluating an MFA $\mathcal{M}$ (resp. Q) at n.

We can identify a class of MFA's, namely, MFA's with a syntactic restriction on FA's called the *split property*, to precisely capture the fragment X_R of regular XPath queries. Let $\mathcal{A} = (K, \Sigma, \delta, s, F)$ be an FA. We call a state q in K a *split state* if (i) q has one incoming and

at most two outgoing ε-transitions; and (ii) if we deleted one outgoing ε-transition, then the FA B induced by all the states in K which were reachable from q through the deleted edge, does not contain a state which is connected to any state outside this B. An FA $\mathcal{A}$ has the *split property* if every AND and NOT state is a split state. An MFA $\mathcal{M} = (\mathcal{N}, \vec{\mathcal{A}})$ has the split property if all the FA's $\mathcal{A}_i$ in $\vec{\mathcal{A}}$ have the split property. Indeed, as shown in [FGJK07], for any $\mathcal{X}_R$ query Q, there exists an equivalent MFA $\mathcal{M}$ with the split property, and vice versa. As a result, MFA's can be used to represent $\mathcal{X}_R$ queries.

7.5 Rewriting Algorithm

We now present an efficient algorithm, called rewrite, for rewriting (regular) XPath queries on arbitrary views into equivalent MFA's on the underlying documents.

Algorithm rewrite. Algorithm rewrite takes as input an $\mathcal{X}_R$ query Q and a view definition $\sigma : D \to D_V$; it returns an MFA $\mathcal{M} = (\mathcal{N}, \vec{\mathcal{A}})$ as output, such that for any XML tree T of D, $\mathcal{M}$ on T yields the same result as Q on $\sigma(T)$. It is based on dynamic programming: for each sub-query Q' of Q and each element type A in D_V, it computes a local translation $\mathsf{rewr}(Q', A)$, i.e., an MFA on D that is equivalent to Q' when Q' is evaluated at any A elements of D_V. The MFA $\mathsf{rewr}(Q', A)$ is constructed inductively, based on structure of Q'. It assembles local translations to obtain $\mathcal{M} = \mathsf{rewr}(Q, r)$, where r is the root type of D_V.

To do this, we use the following variables. (a) A list $\mathcal{L}$ consisting of all the sub-queries of Q, topologically sorted such that for any Q_1, Q_2 in $\mathcal{L}$, Q_1 precedes Q_2 in $\mathcal{L}$ if Q_1 is a sub-query of Q_2. We process the sub-queries in the order of $\mathcal{L}$ such that $\mathsf{rewr}(Q_2, A)$ is defined by composing $\mathsf{rewr}(Q_1, B)$'s for sub-queries Q_1 of Q_2. (b) A list N consisting of all element types in D_V. (c) An MFA $\mathsf{rewr}(Q', A)$ holding the local rewritten MFA $\mathcal{M}(Q', A)$ as mentioned above, in which the SA $\mathcal{N}(Q', A)$ has the form $(K_s, \Sigma_s, \delta_s, s, F, \lambda)$ as described in Section 7.4. (d) A set $\mathsf{eltype}(f)$ for each state f in F, which denotes element types of D_V that are associated with state f when $\mathcal{M}(Q', A)$ is evaluated over an XML tree of D_V (recall the association of states and elements from Example 7.6). In the algorithm we introduce sufficiently many final states such that f is associated with a single type, i.e. $\mathsf{eltype}(f)$ is a singleton set. As will be seen shortly, this is needed when we compute $\mathcal{M}(Q_1/Q_2, A)$ and $\mathcal{M}(Q_1[Q_2], A)$ by composing $\mathcal{M}(Q_1, A)$ and $\mathcal{M}(Q_2, B)$, where B ranges over element types

reached from A via Q_1. We use $N \cup \mathcal{N}'$ to denote the union of two SA's, using the standard NFA union definition.

The algorithm is given in Fig. 7.7. It first compute $\mathcal{L}$ and N (lines 1-2). Then, for each sub-query Q' in the order of $\mathcal{L}$ and each element type A in N, it computes the local translation $\mathcal{M}(Q',A)$ (lines 3–44), bottom-up starting from inner-most sub-query of Q'. The computation is based on the structure of Q' (cases (1)–(6)). We describe three cases below (see Fig. 7.7 for the other cases).

Case (2): $Q' = B$ (lines 8–10). This is the case when the view definition σ is needed. Indeed, following an edge (A,B) in the DTD graph D_v corresponds to following the path $\sigma(A,B)$ in D. Since we may assume w.l.o.g. that $\sigma(A,B)$ is already converted to an MFA, we simply define $\mathsf{rewr}(Q',A)$ to be $\sigma(A,B)$.

Case (6): $Q' = Q_1[Q_2]$ (lines 29–35). Here $\mathsf{rewr}(Q',A)$ is obtained from $\mathsf{rewr}(Q_1,A)$ by annotating each final state f in its SA with a name X, and binding X with the FA computed by Procedure $\mathsf{f\text{-}rewr}(Q_2,B)$. As will be seen shortly, $\mathsf{f\text{-}rewr}(Q_2,B)$ returns an FA representing the filter Q_2 at B elements, and B is the element type $\mathsf{eltype}(f)$ associated with f. There are two cases to consider. If f is already annotated with an FA in $\mathsf{rewr}(Q_1,A)$, then this FA is combined with $\mathsf{f\text{-}rewr}(Q_2,B)$ into a single FA by using a new AND state as the start state of the combined FA, so that both FA's are evaluated at f (lines 33-34). Otherwise a fresh name X is used and is bounded with $\mathsf{f\text{-}rewr}(Q_2,B)$ (line 35).

Case (7): $Q' = (Q_1)^*$ (lines 36–47). By induction, we have already computed $\mathsf{rewr}(Q_1,A)$ for all element types A in D_v. We connect these MFA's together to get $\mathsf{rewr}(Q',A)$ based on reachability information and using a loop. Initially, $\mathsf{rewr}(Q',A)$ is set to $\mathsf{rewr}(Q_1,A)$ (line 36). Let F_s be the set of final states of the SA of $\mathsf{rewr}(Q',A)$ (line 38). For each f in F_s, we add $\mathsf{rewr}(Q_1,\mathsf{eltype}(f))$ to $\mathsf{rewr}(Q',A)$ (if not already present) and connect f via an ε-transition to the initial state of the SA of $\mathsf{rewr}(Q_1,\mathsf{eltype}(f))$. We increment F_s with the final states of the added SA and repeat the above process until F_s does not change and all final states in F_s have been considered (lines 39–44). Here we use a Boolean variable *visited*(B) to ensure that each $\mathsf{rewr}(Q_1,B)$ is included in $\mathsf{rewr}(Q',A)$ at most once.

Procedure f-rewrite**.** The procedure takes as input a filter Q over view DTD D_V and an element type A in D_V, and it returns an equivalent FA $\mathsf{f\text{-}rewr}(Q,A)$ over the document DTD

Algorithm rewrite

Input: a view $\sigma : D \rightarrow D_V$, an $\mathcal{X}_R$ query Q over D_V.
Output: An equivalent MFA over the document DTD.

1. compute the ascending list $\mathcal{L}$ of sub-queries of Q;
2. compute the list N of all the nodes in D_v; /* initialization phase (omitted) */
3. for each Q' in the order of $\mathcal{L}$ do
4. for each A in N do
5. case Q' of /* if not mentioned otherwise, rewr(Q',A) inherits the initial and final states from its building blocks */
6. (1) ε: rewr(Q',A):=$(\mathcal{N}_s, \vec{\mathcal{A}})$, with $\mathcal{N}_s$ consisting of a single
7. state $\{s\}$, eltype$(s) := \{A\}$, and $\vec{\mathcal{A}}$ is empty;
8. (2) B: if B is a child type of A then rewr(Q',A):=$\sigma(A,B)$;
9. F_s:=final states of SA in rewr(Q',A);
10. for each $f \in F_s$ do eltype$(f) := \{B\}$;
11. (3) $\downarrow$: rewr(Q',A):=$\emptyset$; F_s:=$\emptyset$
12. for each child type C of A do
13. rewr(Q',A):=rewr$(Q',A) \cup \sigma(A,C)$;
14. F_s:=$F_s \cup$ final states of SA in rewr(Q',A);
15. for each $f \in$ final states of SA in rewr(Q',A) do eltype$(f) := \{C\}$;
16. (4) Q_1/Q_2: if rewr$(Q_1,A) = \emptyset$ then rewr$(Q',A) := \emptyset$;
17. else rewr(Q',A):=rewr(Q_1,A);
18. F_s := the final states of SA in rewr(Q_1,A);
19. tmp:=$\bigcup_{B \in \text{eltype}(f), f \in F_s}$ rewr(Q_2,B);
20. if tmp= $\emptyset$ then rewr(Q',A):=$\emptyset$
21. else rewr(Q',A):=rewr$(Q',A) \cup$ tmp;
22. for f in F_s do
23. connect f with ε-transition to the initial state of SA in rewr$(Q_2,$eltype$(f))$;
24. final states of SA in rewr(Q',A) are those of NFA in tmp;
25. the initial state of rewr(Q',A) is the initial state of rewr(Q_1,A);
26. (5) $Q_1 \cup Q_2$: rewr(Q',A) := rewr$(Q_1,A) \cup$ rewr(Q_2,A);
27. s_i:=initial state of SA in rewr(Q_i,A), $i = 1,2$;
28. connect new initial state of SA in rewr(Q',A) with ε-transitions to s_1 and s_2;
29. (6) $Q_1[Q_2]$: rewr(Q',A) := rewr(Q_1,A);
30. F_s:=the final states of SA in rewr(Q_1,A);
31. for each $f \in F_s$ do
32. f-rewr$(Q_2,$eltype$(f))$:=f-rewrite$(Q_2,$eltype$(f))$;
33. if $\lambda(f) = X$ s.t. $X = \mathcal{A}$ then /* existing X */
34. connect the initial state of $\mathcal{A}$ and the initial state of f-rewr$(Q_2,$eltype$(f))$ with a new AND state;
35. else $\lambda(f)$:=X; X := f-rewr$(Q_2,$eltype$(f))$; /* X is a fresh distinct name */
36. (7) $(Q_1)^*$: rewr(Q',A):=rewr(Q_1,A);
37. visited(A):=true;
38. F_s:= the final states of rewr(Q_1,A);
39. while next $f \in F_s$ exists do
40. if visited(eltype(f)) = false then
41. rewr(Q',A):=rewr$(Q',A) \cup$ rewr$(Q_1,$eltype$(f))$;
42. visited(eltype(f)):=true;
43. connect f with ε-transition to initial state of rewr$(Q_1,$eltype$(f))$;
44. add final states of rewr$(Q_1,$eltype$(f))$ to F_s;
45. final state set of SA in rewr(Q',A) is $F_s \cup \{s\}$;
46. where s is initial state of SA in rewr(Q_1,A);
47. initial state of SA in rewr(Q',A) is s;
48. return rewr(Q,r);

Figure 7.7: Algorithm for XPath query rewriting

Procedure f-rewrite(Q, A)

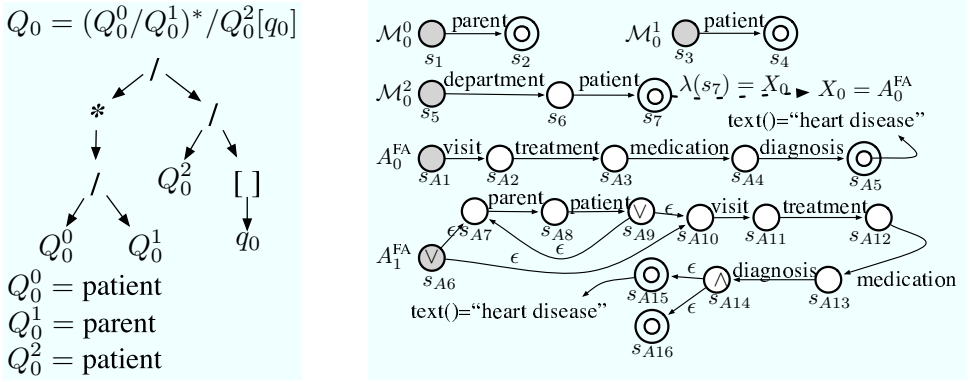
Input: An $\mathcal{X}_R$ query Q over D_V, element type A in D_V.
Output: an equivalent FA over the document DTD.

/* Same structure of algorithm as in rewrite, Q' is a sub-query of Q */
1. case Q' of
2. (1) text='c': f-rewr(Q',A) consists of a single state
3. annotated with text='c';
4. (2) Q_1: f-rewr(Q',A):=mfa2afa(rewr(Q_1,A));
5. (3) $Q_1 \wedge Q_2$: f-rewr(Q',A):=f-rewr(Q_1,A) $\cup$ f-rewr(Q_2,A);
6. add initial AND state connected to initial states
7. of f-rewr(Q_1,A) and f-rewr(Q_2,A);
8. (4) $Q_1 \vee Q_2$: f-rewr(Q',A):=f-rewr(Q_1,A) $\cup$ f-rewr(Q_2,A);
9. add initial OR state connected to initial states
10. of f-rewr(Q_1,A) and f-rewr(Q_2,A);
11. (5) $\neg Q_1$: f-rewr(Q',A):=f-rewr(Q_1,A);
12. add initial NOT state connected to the initial state
13. of f-rewr(Q_1,A);
14. return f-rewr(Q,A);

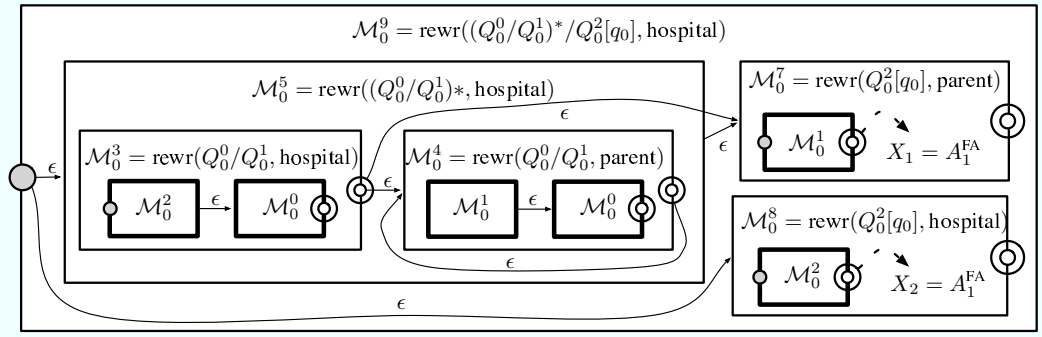
Figure 7.8: Algorithm for regular XPath qualifier rewriting

D as output.

Procedure f-rewrite is given in Fig. 7.8. It constructs an FA again by structural induction on sub-queries Q' of Q (cases 1–5). However, instead of computing the FA's for each sub-query of Q, wherever possible, f-rewrite transforms an MFA, already computed by rewrite for large sub-queries, into an FA. This conversion applies to "path sub-queries" Q' (i.e., of the form p given in Section 7.2), and is done by procedure mfa2afa(rewr(Q',A)) (case 2). To convert rewr(Q',A) into an FA $\mathcal{A}$, we need to ensure the following: (a) each state in $\mathcal{A}$ has at most one outgoing non ε-transition; (b) each state has zero or two outgoing ε-transitions; (c) final states have no outgoing transitions; (d) each state must be assigned a type (K_{op}, K_ℓ or F); and (e) no nested FA's are present. This can all be achieved by inserting new states, making all states having only ε-transitions into OR states, and making states with a labeled



(a) Parse tree of Q_0 (b) Basic rewriting components



(c) Resulted MFA rewriting

Figure 7.9: Rewriting query Q_0 to the corresponding MFA

outgoing transition a K_ℓ state. The nesting of FA's can be avoided as described at the end of Section 7.4.

For the remaining cases (cases 1, 3–5), rewr(Q', A) does the following. For the base cases, f-rewrite creates a single state FA annotated with either *text()*='c' or *position()*=k (case 1). For the Boolean combinations $\wedge$ (resp. $\vee$), f-rewrite connects f-rewr(Q_1, A) and f-rewr(Q_2, A) with a new AND (resp. OR) start state (cases 3–4). Finally, for negation, f-rewrite introduces a new NOT state as the start state (case 5).

Example 7.7: Given query Q_0 of Example 7.6 on the view σ_0 of Example 7.3, assume that we want to compute rewr$(Q_0, \textit{hospital})$. Fig. 7.9(a) shows a simplified parse tree of Q_0. Algorithm rewrite uses this parse tree to inductively build the MFA for Q_0. In more detail, Fig. 7.9(b) shows three MFAs and two FAs that are the basis of the induction of the rewriting of Q_0. Specifically, $\mathcal{M}_0^0$ corresponds to rewr$(\textit{parent}, \textit{patient})$, $\mathcal{M}_0^1$ to rewr$(\textit{patient}, \textit{parent})$

and $\mathcal{M}_0^2$ to rewr$(patient, hospital)$. Notice that the construction of $\mathcal{M}_0^2$ also requires the construction of $\mathcal{A}_0$.

Figure 7.9(c) shows how Algorithm rewrite uses these basic blocks to build inductively the MFA rewr$(Q_0, hospital)$. Specifically, it constructs $\mathcal{M}_0^3 =$ rewr$(Q_0^0/Q_0^1, hospital)$ by concatenating MFA $\mathcal{M}_0^2$ and $\mathcal{M}_0^0$. Then, it constructs $\mathcal{M}_0^5 =$ rewr$((Q_0^0/Q_0^1)^*, hospital)$ by concatenating $\mathcal{M}_0^3$ with $\mathcal{M}_0^4 =$ rewr$(Q_0^0/Q_0^1, parent)$ and adding appropriate ε-transitions for the recursion. Finally, the algorithm considers the rewriting of $Q_0^2[q_0]$ and concatenates this to MFA $\mathcal{M}_0^5$ to compute the final result. □

Similarly rewrite constructs FA's for filters q, with the following features. (a) For a "path sub-queries" Q' (i.e., of the form p given in Section 7.2) of q, rewrite defines its FA in same way as MFA for Q'. (b) For logical connectives $\wedge, \vee$, or $\neg$, rewrite connects inductively obtained FA's by introducing a new logical state, i.e., an AND, OR, or NOT state. (c) For nested filters, i.e., $q = p[q_1]$ where $q_1 = p'[q_1']$, rewrite constructs a *single* FA, rather than nested FA's, for q, by "concatenating" the FA's for p and q_1.

Example 7.8: Consider the filter q_0 in the query Q_0 of Example 7.6. Figure 7.9(b) shows how its FA $\mathcal{A}_1$ is constructed step-wise, by reusing the MFA's $\mathcal{M}_0^0, \mathcal{M}_0^1, \mathcal{M}_0^2$ for path sub-queries, and by concatenating these and "local" FA's to build $\mathcal{A}_0$ and $\mathcal{A}_1$. Note that although q_0 contains a nested filter *text()*='heart disease', the two filters are combined into a single FA and *no "nested" FA's* are required. □

Concluding, we have the following result, which, in contrast to the possible exponential size of the rewritten regular XPath queries, justifies the use of MFA's.

Theorem 7.5.1 *Given a view definition* $\sigma : D \to D_V$ *and an* X_R *query* Q *over* D_V*, Algorithm* rewrite *computes an equivalent* MFA *of size at most* $O(|Q||\sigma||D_V|)$ *over the original document in at most* $O(|Q|^2|\sigma||D_V|^2)$ *time.*

Proof: For each sub-query of Q and element type A in D_V, rewr(Q,A) and f-rewr(Q,A) take at most $O(|Q||\sigma||D_V|)$ time to compute. Since Algorithm rewrite ranges over all sub-queries of Q and all element types in D_V (the nested loop in lines 3–4). □

7.6 Evaluation Algorithm

To make query rewriting a practical approach it is necessary to be able to efficiently evaluate MFA's. We next present an evaluation algorithm for MFA's, referred to as HyPE (Hybrid Pass Evaluation, Fig. 7.10). Algorithm HyPE takes as input a document tree T, a context node n in T and an MFA $\mathcal{M} = (\mathcal{N}, \vec{\mathcal{A}})$; it outputs $n[\![\mathcal{M}]\!]$. The desired result $r[\![\mathcal{M}]\!]$ is obtained by invoking HyPE with the root r of T.

A salient feature of HyPE is that it requires only a *single top-down* pass over the document tree, and a *single* pass over an auxiliary structure, which in most cases is much smaller than the document tree. It employs several pruning strategies in its top-down pass to avoid visiting irrelevant parts of the tree and the computation of irrelevant FA's.

Since any regular XPath query can be transformed into an MFA, HyPE serve as a stand-alone evaluation algorithm for regular XPath, beyond the rewriting context. To the best of our knowledge, HyPE is the first practical algorithm for evaluating regular XPath. Indeed, no practical algorithm has been provided thus far that can be done within a bounded number of tree traversals. For XPath only, a two-pass algorithm was presented in [Koc03]: a bottom-up phase for evaluating filters followed by a top-down phase for selecting nodes. However, it requires a pre-processing step (another scan of the tree) during which the document tree is converted to a special data format (a binary representation of the tree), and the construction of a tree automata which are more complex than MFA's and are possibly large. Algorithm HyPE requires neither pre-processing of the data nor the construction of tree automaton. Moreover, in contrast to HyPE, the two-pass XPath evaluation algorithm may have to evaluate filters at nodes in its first phase, although these nodes will not be accessed in its second phase. As will be verified in Section 7.8, the pruning technique of HyPE speeds up the evaluation of *both* regular XPath and XPath queries.

In a nutshell, HyPE consists of two phases (not to be confused with two passes of the tree T). In the first phase, the tree T is traversed (top-down) depth-first, during which the MFA $\mathcal{M}$ prunes away irrelevant subtrees and identifies which FA's in $\vec{\mathcal{A}}$ need to be evaluated at nodes in the tree. Visited nodes are pushed into a stack $\mathcal{P}$. This stack is used to evaluate the FA's in a synthesized (bottom-up) way. A node is popped from $\mathcal{P}$ once all its related FA's have been evaluated. The size of $\mathcal{P}$ is at most *the depth* of T. During this traversal, HyPE also constructs an auxiliary DAG structure, called cans (for candidate

Algorithm HyPE$(n, T, \mathcal{M})$.

Input: Context node n, tree T, MFA $\mathcal{M}$.
Output: Answer set $n[\![\mathcal{M}]\!]$.

1. Initialize mstates(n), qual(n), and $\mathcal{P} = \{n\}$;
2. cans(n):=PCans$(n,$mstates$(n),$qual$(n))$;
3. Traverse cans(n) starting from set I of cans(n), add
4. visited nodes $\nu(v)$ for vertices in cans(n) to $n[\![\mathcal{M}]\!]$;
5. return $n[\![\mathcal{M}]\!]$;

Procedure PCans$(n, T,$ mstates$(n),$ qual$(n))$

Input: Context node n, tree T, states mstates(n), vector qual(n).
Output: Candidate answers cans(n).

1. if mstates$(n) \neq \emptyset$ or qual$(n) \neq \vec{\emptyset}$ then
2. for each child v of n then
3. $push(v, \mathcal{P})$;
4. mstates(v):=NextNFAStates(mstates$(n), v, \mathcal{N}$);
5. qual(v):=NextAFAStates(qual$(n), v, \vec{\mathcal{A}}$);
6. for each $s \in$ mstates(v), s.t. $\lambda(s) = X_i$, $i \in [1..\kappa]$, do
7. add initial state of $\mathcal{A}_i$ to qual$(v)[i]$;
8. cans(v):=PCans$(v,$mstates$(v),$qual$(v))$;
9. cans(n):=connect mstates(n) to I of cans(v);
10. Set the set I of initial vertices in cans(n) to mstates(n);
11. for each i such that qual$(n)[i] \neq \emptyset$ do
12. fstates$\uparrow(n)[i]$:=PrevAFAStates(fstates$\uparrow(n)[i]$);
13. fstates$\uparrow(n)[i]$:=fstates$\uparrow(n)[i] \cup \{f \in F \mid f$ is true at $n\}$;
14. for each $s \in$ mstates(n) s.t. associated FA is false do
15. Delete s and all its in- and outgoing edges from cans(n);
16. for each final state f of mstates(n) in cans(n) do
17. assign n to f, i.e., $\nu(f) := n$;
18. $pop(n, \mathcal{P})$;
19. if $head(\mathcal{P}) \neq \emptyset$ do
20. u:=$head(\mathcal{P})$;
21. fstates$\uparrow(u)$:=fstates$\uparrow(u) \cup$ fstates$\uparrow(n)$;
22. return cans(n);

Figure 7.10: Evaluation algorithm for MFA's.

answers), representing the history of the run of the selecting automaton $\mathcal{N}$. Vertices in cans will correspond to states in this run for which the associated FA evaluated to true. Moreover, vertices in cans are possible annotated with a node in T which is potentially in the answer set $n[\![\mathcal{M}]\!]$. A node in T associated with a vertex in cans will be in $n[\![\mathcal{M}]\!]$ if this node is reachable from a node in cans corresponding to an initial state of $\mathcal{N}$ at context node n. This allows for distinguishing between potential and real answer nodes in cans. In the second phase, cans is traversed top-down to identify the real answer nodes. The size of cans is typically much smaller than T.

Example 7.9: Consider the MFA $\mathcal{M}_0$ in Fig. 7.5 and the tree T shown in Fig. 7.6. We illustrate how HyPE evaluates $\mathcal{M}_0$ on T through the table in Fig. 7.11. In the figure, we assume that HyPE already traversed, top-down, the left-most patient (node 2) in the tree and we *join* the execution of HyPE at the point where node 9 is considered (the first row in the table). Each row in the table corresponds to a step in the execution of HyPE during which the node n at the head of the stack $\mathcal{P}$ is considered. In the table, we also show (a) $\mathsf{mstates}(n)$, i.e., the ε-closure of states in $\mathcal{N}$ (i.e., the set of states reached by following one or more ε moves), reached by descending to n in T; (b) $\mathsf{qual}(n)$, i.e., a set of states in $\mathcal{A}_0$. If this set is non-empty then n will be involved in the bottom-up evaluation of $\mathcal{A}_0$; and (c) $\mathsf{fstates}{\uparrow}(n)$, i.e., a set of states (and their truth values) of $\mathcal{A}_0$ used in the bottom-up evaluation of $\mathcal{A}_0$. At the bottom of Fig. 7.11, we show the auxiliary structure cans. It is constructed during the traversal of T. We indicate, through boxes, which rows in the table are responsible for the corresponding updates to cans (note that cans is constructed from left to right in Fig. 7.11).

Going back to the figure, the first row of the table indicates two things. First, since s_4 is a final state of $\mathcal{N}$, we know that node 9 is a candidate answer. Second, state s_4 is annotated with $\mathcal{A}_0$ and therefore we need to evaluate $\mathcal{A}_0$ to determine whether node 9 is an actual answer. We *remember* that $\mathcal{A}_0$ needs to be evaluated on node 9 by initializing $\mathsf{qual}(9)$ with the initial states of $\mathcal{A}_0$. Consider now the second row in the table. Node 10 is in the top of $\mathcal{P}$. Furthermore, $\mathsf{mstates}(10)$ is $\{s_1, s_3\}$ and is obtained by calling function NextNFAStates with arguments the $\mathsf{mstates}(9) = \{s_2, s_4\}$ (line 4 in algorithm of Fig. 7.10). Similarly, NextAFAStates computes $\mathsf{qual}(10) = \{s_{A3}\}$ from $\mathsf{qual}(9)$ (line 5 in Fig. 7.10). The fact that $\mathsf{qual}(10)$ is non-empty tells us that node 10 is relevant for the evaluation of $\mathcal{A}_0$. The actual evaluation of $\mathcal{A}_0$ starts when in the head of $\mathcal{P}$ is node 13. At that point, $\mathsf{qual}(13)$ includes the final state of $\mathcal{A}_0$ and from that point on $\mathcal{A}_0$ is evaluated bottom-up. This hybrid

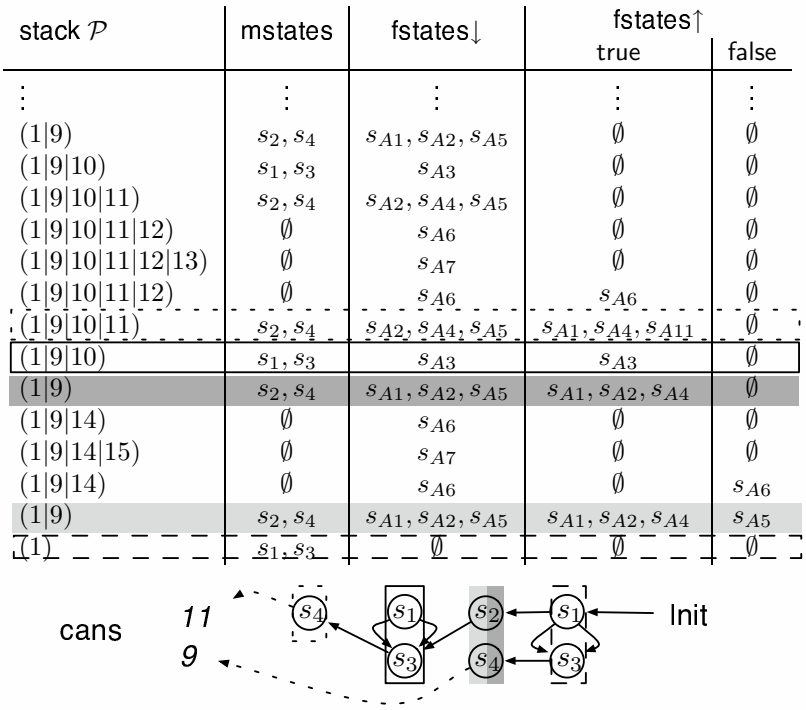


Figure 7.11: HyPE evaluation.

mixing of a top-down with a bottom-up evaluation is the distinguishing characteristic of HyPE. Essentially, HyPE uses the former evaluation type to determine when to initiate the latter. When HyPE returns to $\mathcal{P} = \{1,9\}$ (the dark grey row of the table), the fact that fstates↑(9) includes $\{s_{A1} = \mathsf{true}\}$ indicates that the evaluation of $\mathcal{A}_0$ results in true. Therefore, node 9 is an actual answer. Concerning cans, this is constructed bottom-up. For each node n for which mstates$(n) \neq \emptyset$, mstates(n) is connected to the existing cans, each time the subtree below a child of n has been traversed. For example, when $\mathcal{P} = \{1,9\}$ (dark gray row), mstates(9) is connected (using the transitions in $\mathcal{M}_0$) to the cans structure to its left. At this point, notice that by following the path s_2, s_3, s_4 we reach node 11 in T. Furthermore, through the new state s_4 node 9 is also reachable. When the construction of cans is completed (row with dashed box), a traversal of cans starting from the Init nodes shows that nodes 9 and 11 are still reachable and hence are in the answer of $\mathcal{M}_0$ on T. □

Complexity. The complexity of HyPE is determined by that of PCans (for constructing cans) and the traversal of cans. PCans needs for each context node n at most $O(|\mathcal{M}|)$ time. Moreover, connecting and updating cans takes at most $O(|\mathcal{M}|)$ time as well. Hence, the

overall time complexity of PCans is $O(|T||\mathcal{M}|)$. Moreover, PCans requires a single scan of the input document T and cans. The space requirement of PCans is dominated by the size of cans, which, although in the worst case is $O(|T||\mathcal{M}|)$, is typically much smaller than $|T|$. Traversing cans takes again $O(|T||\mathcal{M}|)$ time in the worst case. As a consequence:

Theorem 7.6.1 *Given an* MFA $\mathcal{M}$ *and tree* T, HyPE *computes* $r[\![\mathcal{M}]\!]$ *in at most* $O(|T||\mathcal{M}|)$ *time and space.*

Using the evaluation algorithm together with the rewriting algorithm, we obtain a complete practical method for answering queries on (virtual) views. The overall complexity of our method follows from Theorems 7.5.1 and 7.6.1.

Theorem 7.6.2 *Given an* $\mathcal{X}_R$ *query* Q *on a view of an* XML *source* T*, our query answering method returns the answer to* Q *in* $O(|Q|^2|\sigma||D_V|^2 + |Q||\sigma||D_V||T|)$ *time.*

The size $|T|$ of the document is dominant and is typically much larger than the size $|D_V|$ of the view DTD and the size $|\sigma|$ of the view definition σ; when only $|T|$ is concerned (e.g., if D_V and σ are fixed as commonly encountered in practice), our method answers queries in *linear-time* (data complexity), and in quadratic combined complexity.

Comparison with materialized approaches. In addition to query rewriting, there are another two competing approaches for answering queries on the views:

The first one is to materialize the view through a pre-processing step. Any queries on the view are then answered by evaluating them over the pre-materialized view directly. In this approach, the query answering step has a $|Q||\sigma||D_V||T|$ time complexity. However, as mentioned earlier, in terms of both time and space, it is often prohibitive expensive to materialize and maintain a large number of views. In XML security context, it is common to define a large number of views to provide access to each user group.

The second approach is to materialize the view on the fly when a query is posed. This run-time materialization approach avoids the space wasted by multiple copies of the data and the time wasted by view maintenance in response to modifications of the underlying XML document. The query answering has $O(|Q||\sigma||D_V||T|)$ time complexity. However, in practice, the query and view definition are usually far smaller than the XML document. The query rewriting step is independent to the XML document; while the materialization

step needs to traverse the XML document multiple passes. This approach will inevitably waste computations to generate and store the part of views which is irrelevant to answer the query.

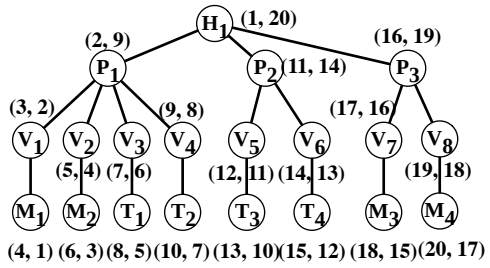
7.7 Optimizing Regular XPath Evaluation

Although HyPE already performs well in practice (see Section 7.8), we developed a novel index structure which enables HyPE to skip even more subtrees. In the following, we denote by OptHyPE the version of HyPE which is built on top of the index, and by OptHyPE-C the version of HyPE which uses a compressed version of the index.

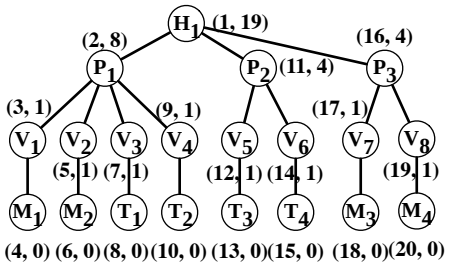
Given a query Q over a tree T, the secure sub-framework employs a novel index structure on T to decide whether HyPE can skip from visiting certain sub-trees of T. The introduced index structure is capable of summarizing, at each node u, information regarding all the nodes in the subtree that is rooted at u. In what follows, we first present the index and then describe how it is used in optimization. We note that both the index structure and our optimization technique are generic enough to be applicable in other contexts or optimization efforts, not just for rewritten queries (MFA's).

7.7.1 The Type-Aware XML (TAX) index

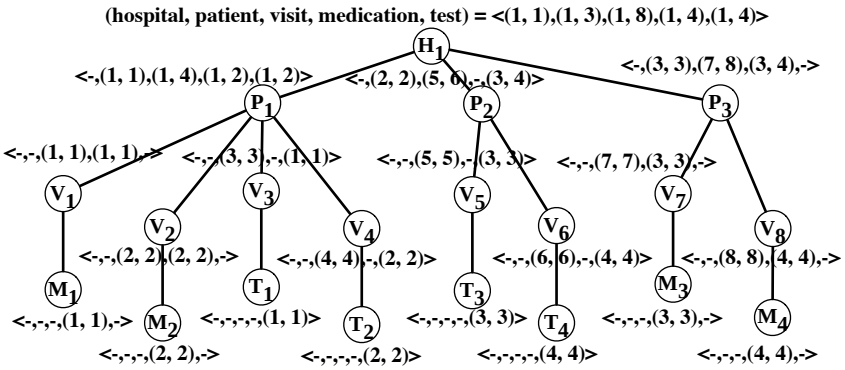
Of major concern in the optimization of XPath queries is to minimize the cost of the '//' operator. To this end, various number indexing structures have been proposed that, given two nodes u and w, they can answer in constant time whether node u is an ancestor of w. One such scheme uses the pair of pre/post-order tree traversal numbers to annotate each node [Die82]. Figure 7.12(a) shows an example of the index over a tree that conforms to a simplified version of our *hospital* DTD. To save space, the simplified DTD only considers *hospitals*, their *patient*s, and each *patient* has *visit*s that involve either a *test* or a *medication*. In this scheme, a node u is an ancestor of w if u occurs before w in the preorder traversal and after w in the postorder traversal. An alternative index was proposed in [LM01] in which a node is annotated with the pair of preorder traversal and *range* numbers, where the latter is the maximum number of descendants of the node. Figure 7.12(b) shows an example of the order/range scheme, on the same tree as in Fig. 7.12(a). In the order/range index, u is



(a) Pre/Post order scheme



(b) Order/Range scheme



(c) The TAX-index scheme

Figure 7.12: Three numbering indexing schemes.

an ancestor of w if the preorder of w is larger than that of u and smaller that the sum of the order of u and its range.

Existing number indexing schemes assume a *random access* evaluation algorithms [MW99, LM01] and, therefore, are not useful for algorithms like HyPE that follow a strict top-down evaluation order. To see this, consider how random access evaluation algorithms work. Such algorithms typically decompose the input query Q into a set of sub-queries, evaluate each sub-query independently, and piece together the results of the different sub-queries by means of the index. For example, a query that retrieves all the tests of a particular patient, say patient P_1 in the figure, might involve (1) retrieving the *patient* node; (2) independently retrieving all *test* nodes T_i, $1 \leq i \leq 4$; (3) using the index to find all the *test* nodes that are descendants of P_1, i.e., nodes T_1 and T_2, without accessing any intermediate *visit* nodes. Given that in our case HyPE follows a strict top-down order of evaluation and it deals with regular XPath queries with (possibly nested) Kleene closures, the ancestor/descendant

relation provided by the index is not very useful.

Another, rather surprising, thing to notice about existing number indexing schemes is that the index of a tree T provides minimal information about the tree it indexes. Consider, for example, the index entry of node H_1 in Fig. 7.12(a). As long as the sub-tree rooted at H_1 consists of 19 nodes, the index entry of H_1 remains unchanged. Just by looking at the index of H_1, we cannot tell whether this is the root of a tree with a single *patient* and eight recorded *visit*s or it has the structure of the tree shown in the figure. This does not meet our expectation that an index provides at least some information about the indexed item, in XML and in general.

In response to this we introduce a novel indexing structure that can be used *both* in strict *top-down evaluation* algorithms, like HyPE, and in *random access evaluation* algorithms. The index provides, at each node u, an accurate summary of the nodes that are in the sub-tree rooted at u. Central to the summarization process is the simple observation that different nodes in the tree have different types. To the best of our knowledge, all number indexing schemes in the literature are *type-agnostic*, that is, they assigns numbers to nodes but ignore the fact that different nodes have different types. However, it is natural to index the nodes of each type separately and it is not a coincidence that in relational databases we usually index each relation attribute (type) independently and we do not build one big index for the whole relation.

We next present the Type-Aware XML index, or TAX-index for short. A TAX-index essentially encapsulates as many indexes as there are types in the DTD. In the TAX-index, for each node u in a tree T we maintain a vector V_u of size $|Ele|$, where Ele is the set of types in the DTD D of T. We use $V_u(E)$ to denote the element in vector V_u for type $E \in Ele$. Each such element contains a pair of numbers and thus each node requires $O(|Ele|)$ space (we show how to compress the index shortly). Sometimes, an element is left without value. In that case we put a dash in its position. Figure 7.12(c) shows an example of the index, where $|Ele| = 5$ and the values of the vector are shown for each node.

We now explain how we assign values to the vector elements and the meaning of this assignment. We assign identifiers to nodes of different types independently by numbering all the nodes of a type in a preorder traversal of tree T. Consider a node u of type E and assume that u is the i^{th} node of type E encountered during the traversal. Then, $V_u(E)[0] = i$, where $V_u(E)[0]$ is the first entry of the $V_n(E)$ element. The value of the second entry in the

element is explained later. In Fig. 7.12(c), $V_{P_2}(patient)[0] = 2$ while $V_{V_2}(visit)[0] = 2$ Now, consider element $V_u(E')$ for node u, for any type E' other than E. In this element, we store the smallest and largest identifier of nodes that are of type E' and belong to the subtree of T rooted at u. In the figure, node P_1 has $V_{P_1}(visit) = (1,4)$ to indicate that the *visit* nodes with identifiers from 1 to 4 are its descendants. Similarly, $V_{P_1}(medication) = (1,2)$ to indicate that *medication* nodes with identifiers 1 and 2 are descendants of the P_1 node. One more detail remains, concerning the value of the second entry in $V_u(E)$. In this position, we store the largest identifier of a node of type E that is a descendant of u. If the DTD is recursive, it is possible that nodes of the same type are descendants of each other. Algorithm buildTAXIndex (omitted due to space limitations) computes the vectors V_u for all the nodes u of a tree T via a single traversal of the tree. In terms of space, a naive strategy would require $O(|T||Ele|)$ space. However, we can compress substantially the vector of each node. Indeed, for a node u of type E, we only need to allocate space in the vector for the types that can be descendants of E. Through static (offline) analysis of the DTD, we can determine which these types are for each E. Using this optimization, for the TAX-index in Fig. 7.12(c), we can save the space for almost all the dash ("-") entries. Indeed, our experiments show that, in spite of its added-value, the space requirements of a compressed TAX-index are at most three times that of the corresponding order/range index over the same tree. In the following section, we show how we can go one step further to compress the TAX-index even more.

A TAX-index summarizes, at each node, information regarding the subtree that is rooted at that node. This is used in the next section to optimize the evaluation of $\mathcal{X}_R$ queries. The following proposition shows that a TAX-index can do more, namely, it can also be used to answer ancestor/descendant queries.

Proposition 7.7.1: *For any two nodes n and n' of a tree T, n is an ancestor of n' iff for each $E \in Ele$, $V_n(E)[0] \leq V_{n'}(E)[0]$ and $V_n(E)[1] \geq V_{n'}(E)[1]$.* □

7.7.2 The Optimization Algorithm

Our optimization algorithm, called OptHyPE, is built on top of the HyPE Algorithm. Algorithm OptHyPE uses the TAX-index to reduce both the number of tree nodes visited by the selection automaton $\mathcal{N}$ and the number of filters evaluated by the FA's. To do this, the algorithm first assumes that each state of both the selection SA $\mathcal{N}$ and the FA's is annotated

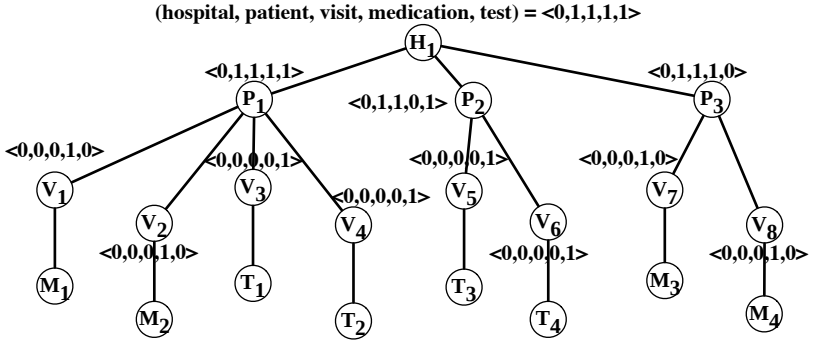


Figure 7.13: The TAXbit-index scheme

with the types of the elements that can reach this state. We are mainly interested in the annotation of final states which identify, in the case of the SA $\mathcal{N}$, the set Ele^N of element types of nodes that can appear in the answer set.

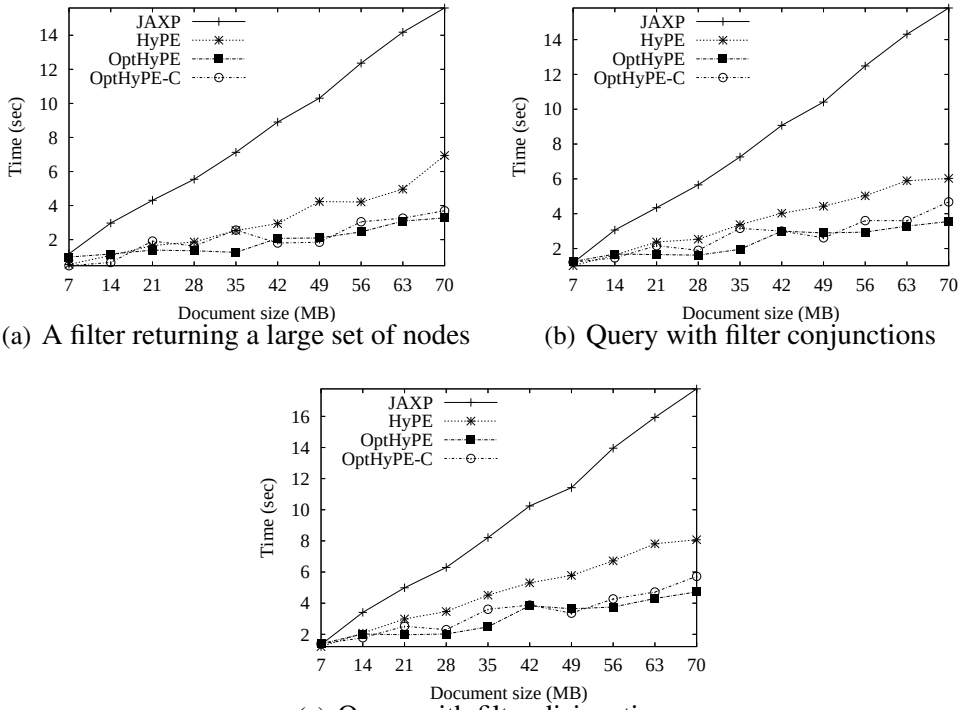
Now, consider a query $Q = hospital/patient/visit/medication$, which returns all the medication of the hospital patients. Then, $Ele^N(Q) = \{medication\}$. Using HyPE, we need to access all the nodes in the tree shown in Fig. 7.12(c) in order to return the four medication leaf nodes. However, we can use the information in the TAX-index to reduce the number of node accesses as follows. Consider the phase in the HyPE during which we have already visited the two left-most subtrees of the *patient* node P_1. At this point, node P_1 is at the top of the stack and the two left-most *medication* leaf nodes M_1 and M_2 are already in the potential answer set. Under normal execution, HyPE will add in the stack node V_3 in order to continue the evaluation of the remaining subtree that is rooted at P_1. However, we know from $Ele^N(Q)$ that we are looking for *medication* nodes and we also know that we already retrieved two such nodes in the subtree of P_1. Furthermore, from the TAX-index entry of P_1, we know that P_1 has only two such nodes as descendants. Thus, we need not evaluate any other part of the subtree of P_1 since we are sure that no more *medication* nodes exist. This observation is used by our optimization algorithm to save four (unnecessary) node accesses. Using similar reasoning, we save four more node accesses at node P_2 since no *medication* nodes are present in its subtree. Overall, our optimization algorithm performs, in this example, 40% less node accesses than HyPE.

Interestingly enough, the same idea works for the evaluation of filters. For example, consider the following query Q' that returns all the *patient*s for which there is some test,

that is, $Q' = hospital/patient[visit/test]$. We know that for the filter automaton $\mathcal{A}$, $Ele^{\mathcal{A}} = \{test\}$. Again, using HyPE we need to evaluate the filter in 16 nodes (all the nodes in the subtrees that are rooted at *patient* nodes). However, given the TAX-index entries for nodes V_1 and V_2, we know that we do not need to visit any of their descendants since there are no *test* nodes there. This observation is used by our optimization algorithm to save two node accesses (the M_1 and M_2 nodes). Using similar reasoning, we save four more node accesses by not evaluating the filter in the subtree rooted at node P_3. Overall, our optimization algorithm performs, in this example, 37.5% less node accesses than HyPE.

Briefly, we describe the implementation of OptHyPE (which is an extension of HyPE and is omitted due to lack of space). We extend HyPE to maintain a global vector GV which stores the summary of the visited nodes. For example, while evaluating query Q above, and after visiting the two left-most subtrees of node P_1, the vector is $GV = \langle(1,1),(1,1),(1,2),(1,2),-\rangle$, while GV is equal to $\langle(1,1),(1,3),(1,6),(1,2),(1,4)\rangle$ after visiting node P_3 and before any of its descendants is accessed. During evaluation in OptHyPE, vector GV is compared with the vector of the node at the top of the stack, for example with that of node P_1. Since we are looking for *medication* nodes, and since $GV(medication) = V_{\mathbf{P_1}}(medication)$ (we already visited all the *medication* descendants of P_1), algorithm OptHyPE skips from visiting the remaining subtree of P_1. The vector of P_1 is also used to update GV with information regarding the unvisited parts of the tree.

There is an alternative implementation of OptHyPE that results in significant space savings, in terms of the size of the index used, but may result in some additional node accesses. Briefly, notice that in our optimization algorithm it often suffices to know that a descendant of a particular type exists, or not. Since we are not interested (at least in HyPE) in ancestor/descendant queries, we can use a variation of the TAX-index, called TAXbit-index and shown in Fig. 7.13, which only uses a single bit in entry $V_u(E)$ of a node u to indicate whether node u has a descendant of type E. It is not hard to see that we can still use the index while evaluating the query Q above. Assuming that we have already visited the two left-most subtrees of P_1, we need to descent to node V_3 before we realize that no *medication* nodes exist there. We still save the cost of visiting the subtree rooted at P_2 since we already know that no *medication* nodes exist there. Overall, for this example, we perform 37.5% less node accesses than HyPE.



(a) A filter returning a large set of nodes (b) Query with filter conjunctions

(c) Query with filter disjunctions

Figure 7.14: XPath query evaluation times

7.8 Experimental Study

We have developed a prototype system SMOQE [FGJK06] supporting MFA's and algorithms rewrite and HyPE (and its variants OptHyPE and OptHyPE-C). In our experiments, we focused on the most time-consuming module of SMOQE, i.e., the query evaluator. The experiments were conducted on a dual 2.3GHz Apple Xserve with 4GB of memory. For the generation of our datasets, we used ToXGene [BMKL02]. We generated XML documents that conform to our recursive hospital DTD shown in Fig. 7.1, with sizes ranging from 7MB to 70MB, in 7MB increments. Each increment roughly corresponds to adding the medical history of 10,000 patients to our document tree. Therefore, the largest document stores the medical history of approximately 100,000 patients. The maximal depth of the trees is 13. The generated data consist mainly of element nodes, and to a lesser extent of text nodes. Therefore, the size of the document has a direct impact on query evaluation. For example, our smallest document (7MB) consists of 303,714 element nodes vs 151,187 text nodes. The text nodes are used to increase the selectivity of queries but their size is kept to

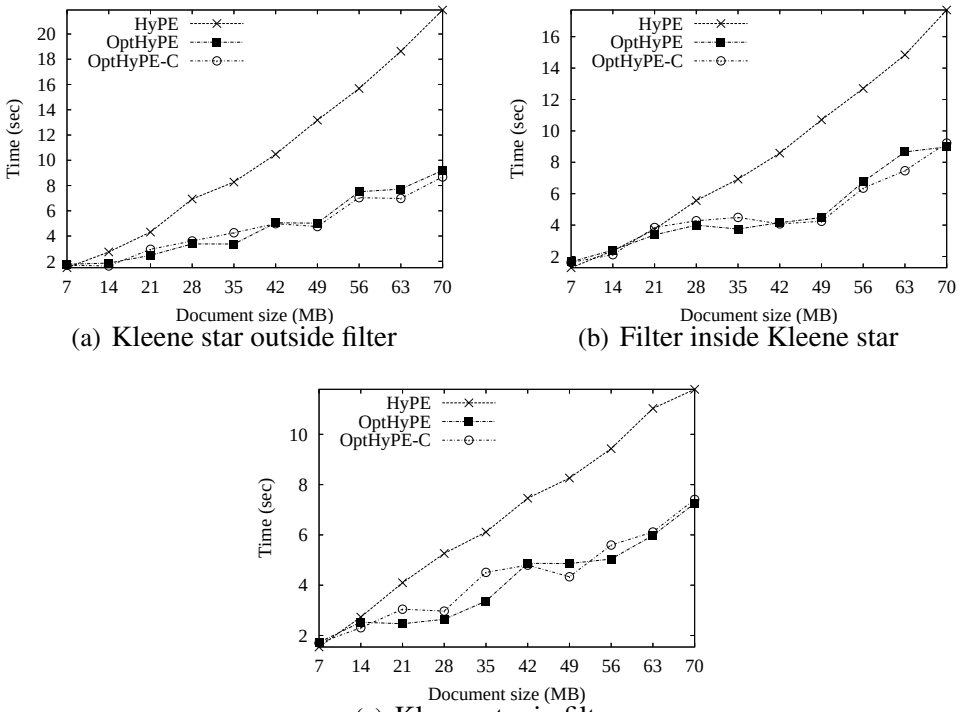


Figure 7.15: regular XPath query evaluation times

a minimum (so as not to increase the document size).

Using the generated document trees, we conducted two sets of experiments, one regarding XPath evaluation, the other regarding regular XPath. The reported times are averaged over at least 5 runs of each experiment.

Evaluating XPath Queries. Since regular XPath subsumes XPath, we investigate the performance of HyPE and its variants for the evaluation of XPath queries.

We compared our performance with that of the Java API for XML Processing Reference Implementation (JAXP RI 1.3), which relies on XERCES and XALAN [XX]. We also compared with JAXP-COMPILE, a version of JAXP that pre-compiles the input query and converts it into a set of Java classes. The two JAXP versions had similar performance and thus we only report one of them.

We ran various types of XPath queries with simple filters on data values, unions of queries, and Boolean combinations of filters. Figure 7.14 shows the evaluation time for three different types of XPath queries. We show the evaluation time both for queries with

result sizes of a few hundreds of nodes (Figures 7.14(b) and (c)) and queries that return a few thousands of nodes (Fig. 7.14(a)). For each query type, we report the evaluation time for JAXP, HyPE, OptHyPE and OptHyPE-C. The figures show clearly that our algorithm consistently outperform JAXP by a factor of *three* for HyPE, and *four* for OptHyPE and OptHyPE-C. We also observe that in most cases, both optimized versions of HyPE run almost twice as fast as HyPE. Note as well that the performance of OptHyPE-C is almost identical to that of OptHyPE (while OptHyPE-C uses a compressed index).

Evaluating Regular XPath Queries. The second set of experiments investigated the performance of evaluating regular XPath queries with the different versions of HyPE. Existing alternatives rely on a translation of regular XPath into a more powerful query language like XQuery. We conducted a series of experiments following this approach. Specifically, we translated several regular XPath queries into XQuery and evaluated them in GALAX (*http://db.bell-labs.com/galax*). These experiments consistently showed that the queries in XQuery required considerably more time than their regular XPath counterparts. As a result we omit GALAX from our discussion because even for a simple regular XPath query on the smallest used document tree, GALAX needed more time than HyPE for the same query on the largest tree. Hence, we only focus on the relative performance of our algorithm.

We ran different types of regular XPath queries that involve Kleene star outside a filter, inside a filter, filters inside Kleene stars and combinations thereof. Figure 7.15 reports the evaluation time for three of these queries. The overall conclusion is consistent with our observations regarding XPath queries. Indeed, OptHyPE and OptHyPE-C show considerable improvement over HyPE.

An interesting observation is that HyPE prunes a substantial number of element nodes. Specifically, HyPE (resp. OptHyPE) prunes, on average, 78.2% (resp. 88%) of the element nodes for our example queries.

7.9 Related Work

There has been a host of work on rewriting queries posed on XML views to relational queries on top of RDBMS (e.g., [SKS+01b, FKMT02]). Such XML views originate in either the context of XML *publishing*, where XML views are obtained from relational data, or

in the context of XML *storage*, where XML views reflect XML data stored in a relational database. In both contexts, XML queries on the XML view need to be translated into SQL. Even in this setting, recursion in the view DTD makes the translation challenging. As observed by [KKN04], most of the existing approaches cannot translate recursive queries over recursive views (two exceptions are [SKS$^+$01b, FYL$^+$05]).

There has been little work on query rewriting for XML views in the native XML setting where one does not rely on any RDBMS, i.e., the setting considered in this chapter. [PA05] concentrates on views in XML integration context, while [FCG04] and [BF05] in XML security context. [PA05] investigates the query answering on XML views defined in local-as-view (LAV) approach with constraints on global schema. The view and the query are specified in a so called prefix-selection query language which is base on homomorphism between trees that preserves root, parent-child relationships and labeling. The filters in XPath can be expressed in the language, but recursive axes such as descendant axis can not. Polynomial time (data complexity) query answering algorithm is developed based on constructing a weak representation system to represent all legal XML instance over global schema under the view definition (i.e. the mappings from global schema to source schema as well as the constraints on global schema). [BF05] studies the closure properties and algorithms for the query rewriting (called query composition there) of several fragments of a subtree query language for views defined in global-as-view (GAV) approach. The language is defined by modifying the semantics of XPath fragments. The largest fragment studied in [BF05] is syntactically comparable to the XPath fragment $\mathcal{X}$ studied in this chapter with extension to upward axes. The motivation of their language is to give a convenient way for specifying certain subtree queries. It can not express the views defined in this chapter which hide certain ancestors of some nodes in the view — the views defined by [BF05] always have the same root-to-leaf paths as the underlying document. Their query rewriting algorithm runs in polynomial time in the size of the queries, under the assumption of normalization (for un-normalized queries, there is a provable exponential blow-up). [FCG04] studies the query rewriting algorithms for the views defined similarly as ours. It shows that $\mathcal{X}$ is closed under query rewriting for *non-recursive* XML views. Our rewriting algorithm in this chapter gives a practical solution to rewriting queries in XPath and its extension regular XPath over recursive XML views which can hide arbitrary XML nodes.

The research on XML access control enforcement could be classified as either static

mechanism which enforces access policies at compile-time of the query evaluation or dynamic mechanism which enforces them at run-time of the query evaluation. In a compile-time approach, the access policies are embedded into queries. The access control enforcement is typically achieved by either *query filtering* where the part of queries that returns unauthorized information is filtered out, or *query rewriting* where the accessible information is explicit defined for authorized users as virtual views. [MTKH06, LLLL04] take query filtering approach. Both of them use automata to represent access policies. In [LLLL04] the policies are embedded into the queries by evaluating the queries on the automata that represent the policies. In [MTKH06], besides the policies, the queries and schemas, if available, are also represented by automata. Then the automata represented queries are compared with the automata represented policies and schemas. If the queries are partially granted, a run-time checking is still needed. As mentioned in Section 7.1, [FCG04] follows query rewriting approach. A view definition and a view schema are explicitly derived from the security policies. The query on the view is then unfolded to incorporate the view definition.

In a run-time approach, the access policies are associated with XML documents. A naïve way to achieve the association is to annotate (also called label), each node in XML documents with security properties such as the user groups/roles that can access the node. These annotated documents could be prohibitively large because the user groups/roles and access actions are appended in every nodes. A host of research [YSLJ04, JF05, ZZSZ07] focuses on compressing the annotated documents and supporting queries on them. The compressing is usually done by utilizing *access locality*. Access locality is the property that the adjacent nodes in an XML tree tend to have the same access policies. Thus, it is not necessary to annotate every node in an XML tree and the annotated documents could be represented compactly. In [YSLJ04, JF05], the compact representation is called Compressed Accessibility Maps (CAMs) where the adjacency is defined by the ancestor-descendant relationship. In [ZZSZ07], it is called Document Ordered Labelling (DOL), where the adjacency is defined by document order. Although the compression reduced the space consumption, the mixture of XML instance and security properties and the time required to compute the compression are still disadvantages of the run-time approach. In many cases, the compile-time approach is preferred because the XML documents, which are usually large in database applications, are not touched. A critical problem in the compile-

time approach is query rewriting on XML views, which is a focus of this chapter. More work on XML access control can be found in a survey [FM04].

In [Mar04b], regular XPath was introduced and it was shown that a regular XPath query Q can be evaluated over an XML tree T in $O(|Q||T|)$ time, requiring multiple passes over the document tree. A two-pass algorithm for XPath was developed in [Koc03], but it cannot be easily extended to deal with the Kleene star. As already observed in Section 7.6, even when only XPath is concerned, our evaluation algorithm, HyPE, does not need a pre-processing step (another scan of T) that is required by the algorithm of [Koc03], and is more effective in pruning irrelevant nodes when traversing T, among other things.

Several automaton formalisms were proposed for processing multiple XPath queries on streaming XML (e.g. [DFFT02, GGM$^+$04]). The idea of AFA was explored by [GGM$^+$04] for evaluating XPath filters. However, no previous work has attempted to characterize regular XPath in terms of both NFA and AFA in an integrated automaton.

Another line of research concerns view-based *query rewriting* and *answering* (see [Hal01] for a survey). Here, given a set of (materialized) views and a query Q on the underlying database, the goal is to answer Q solely on the basis of the views. The problem we consider here is the *opposite scenario* where the query Q is posed on the view, and it is to find a rewriting Q' of Q on the underlying document.

Chapter 8

Conclusions and Future Directions

With the increasing complexities of the data in real world organizations and the advancing technologies to manage the data, information systems need to be enhanced in several dimensions. For instance, in data dimension, the systems need to cope with both structured data and semi-structured data. In service dimension, beyond storing and querying large volume of data, the systems need to provide functionalities to improve the quality of the data, integrate the data from heterogeneous sources and protect the data against unauthorized access. In response to these challenges, this thesis presents a comprehensive framework, referred to as CLINSE, to clean, integrate and secure data by leveraging both relational and XML data management techniques.

In CLINSE, three sub-frameworks have been proposed. First, the inconsistencies in the data residing in each relational data source are detected and repaired in the data cleaning sub-framework. Second, the relational data is published into XML format and integrated with other XML data sources guided by a predefined schema in the data integration sub-framework. At last, the integrated XML data is protected by a security sub-framework which hides the integrated data, but exposes a virtual XML view for each user group and supports query answering on these views.

Data cleaning sub-framework. To clean the data stored in relational databases, the thesis has introduced CFDs as an extension of FDs, and shown that CFDs are capable of capturing inconsistencies beyond what traditional FDs can detect. To apply CFDs in data cleaning, SQL-based techniques for detecting violations of CFDs have been proposed and experimentally evaluated. These results, together with the static analysis reported in [BFG$^+$07],

establish a constraint-based model for data cleaning.

In CLINSE, based on CFDs, a sub-framework for improving data quality has been proposed. It is shown that while CFDs are more appropriate for data cleaning than traditional FDs, they make our lives harder when developing (semi-)automated data-cleaning methods based on CFDs. Indeed, previous methods based on FDs may not even terminate when applied to CFDs. It is shown that based on CFDs, the problem for finding optimal repairs and the problem for incrementally finding optimal repairs are both NP-complete. In light of these intractability results, heuristic algorithms for both problems have been developed in CLINSE framework. Moreover, their effectiveness and efficiency in improving the consistency of the data have been experimentally verified. This work is the first effort to (incrementally) clean data based on conditional constraints.

Data integration sub-framework. To integrate data, a novel language, XIGs, has been proposed for specifying XML integration. XIGs automatically support conformance to a target DTD. They allow one to build a large, complex integration via composition of component XIGs. Novel optimization algorithms for evaluating XIGs have also been developed. These lead to a design tool and a user/application-level interface for XQuery to facilitate schema-directed XML integration.

Data security sub-framework. To secure the XML data, a sub-framework for efficiently answering regular XPath queries posed on possibly recursively defined XML views has been provided. On the theoretical side, results have been established for the closure property and complexity of rewriting (regular) XPath queries on views into (regular) XPath queries on the source. On the practical side, a practical approach has been proposed for query rewriting, by using MFA as an intermediate representation of rewritten regular XPath queries. The novelty of the approach consists in (a) an algorithm for rewriting regular XPath queries on XML views to equivalent MFA on the source, and (b) an efficient evaluation algorithm for MFA. These yield an effective method for answering queries posed on XML views of XML data, and are useful in enforcing XML access control, among other things. Furthermore, the evaluation algorithm is among the first for efficiently processing regular XPath queries. A prototype system supporting all these algorithms has been fully implemented, and the experimental results verified the efficiency of these techniques.

There is much more to be done.

XML data cleaning. In the current framework, only the data in relational sources is cleaned before integration. However, the data in other sources, especially XML sources, may contain errors and need to be cleaned too. More importantly, the data integration process may also introduce dirty data due to the mis-translation and incompatibility of the semantics of the source data. Therefore, XML data cleaning is definitely needed in this framework. Beyond CLINSE framework, XML data cleaning tools are valuable in cleaning the data extracted from the Web, such as address data. Although the constraints for XML data cleaning could be defined as assertions in Schematron [ISO06a], how to check the consistencies of these assertions and use them to detect and repair XML data are still open problems.

Other conditional constraints for relational data. To clean relational data, constraints beyond CFDs are certainly needed. For example, data cleaning based on both CFDs and conditional inclusion dependencies, which are defined along the same lines as CFDs, needs to be studied. The static analysis of these conditional dependencies becomes, however, more intriguing. In particular, the consistency and implication problems for these conditional constraints become undecidable. To cope with this it is necessary to find effective and efficient heuristic algorithms for the consistency and implication analyses of these conditional constraints.

Improve constraint-based data cleaning by profiling the data. Automated methods for discovering CFDs and conditional inclusion dependencies are certainly an interesting topic. It is nontrivial to identify all sensible pattern tuples without over-populating pattern tableaux. Probably, a more general question is whether constraint-based data cleaning and data profiling could be combined to provide better results. For example, in constraint-based data cleaning, the inconsistent data may also contain clean data. Currently, cost models are used to decide which part of the inconsistent data is dirty. On the other hand, the outliers discovered in data profiling could be correct data. However, if part of the inconsistent data detected by constraint-based data cleaning is among these outliers, it is more likely to be dirty. Moreover, the repair suggestions in data profiling could be validated by the constraints. Although such mutual verification is feasible in principle, its effects in practice and the choice of constraints and outlier models are topics to be explored.

XML views on heterogeneous data. In CLINSE framework, XIGs are used to specify

XML views over XML data. The data under other models needs to be published into XML format before the integration. A simplification of this process would be to incorporate XML publishing features into XIGs. Extending XIGs to allow both XQuery and SQL to be associated with productions of the target DTDs would enable XIGs to define XML views over heterogeneous data, but how to cope with both the tree valued attributes and tuple valued attributes, and how to optimize the evaluation of the extended XIGs are challenging problems. Another direction for improving XIGs is to identify practical XQuery fragments that allow efficient optimization techniques and termination analyses for XIGs.

XML Query rewriting in other contexts. In this thesis, (regular) XPath query rewriting in security context is studied. It is interesting to extend this work to other contexts and other XML query languages, such as, how to rewrite queries over XML views of multiple XML data sources as found in data integration, and how to extend the rewriting algorithms to handle queries and views specified in XQuery.

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